

Cr<sub>2</sub>Nb-BASED ALLOY DEVELOPMENT

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## ABSTRACT

Alloys of Cr-Cr<sub>2</sub>Nb with exceptionally high strength at 1200°C have been developed. However, these compositions suffer from limited ductility and toughness at room temperature. Despite improvements from processing modifications, as-fabricated defects still limit room temperature mechanical behavior. In contrast, an alloy system with only a small mismatch of the coefficients of thermal expansion of the two phases, Cr-Cr<sub>2</sub>Zr, showed good fabricability. However, these alloys are weaker than Cr-Cr<sub>2</sub>Nb compositions at high temperatures and have poor oxidation resistance. Silicide coatings can provide high-temperature oxidation and sulfidation protection of these alloys. Improvements in room temperature mechanical properties of Laves-phase-strengthened alloys will rely on further development based on increasing the ductility of the matrix phase by impurity control and compositional modifications.

## INTRODUCTION

The objective of this work is to develop a new generation of structural materials based on intermetallic alloys for use at high temperatures in advanced fossil energy conversion systems. Target applications of such ultrahigh strength alloys include hot components (for example, air heat exchangers) in advanced energy conversion systems and heat engines. However, these materials may also find use as wear-resistant parts in coal handling systems (for example, nozzles), drill bits for oil/gas wells, and valve guides in diesel engines.

One potential class of such alloys is that based on Cr-Cr<sub>2</sub>Nb alloys. The intermetallic phase, Cr<sub>2</sub>Nb, with a complex cubic structure (C-15)<sup>1,2</sup> has been selected for initial development because of its high melting point (1770°C),<sup>2-4</sup> relatively low material density (7.7 g/cm<sup>3</sup>),<sup>5</sup> and excellent high-temperature strength (at 1000 to 1250°C).<sup>6,7</sup> This intermetallic phase, like many other Laves phases, has a wide range of compositional

homogeneity<sup>2,4</sup> suggesting the possibility of improving its mechanical and metallurgical properties by alloying additions.

The major engineering concern with  $\text{Cr}_2\text{Nb}$  and other  $\text{A}_2\text{B}$  Laves phases is their poor fracture toughness and fracture resistance at ambient temperatures.<sup>3,6-9</sup> The single-phase  $\text{Cr}_2\text{Nb}$  is very hard (~800 DPH) and brittle at room temperature.<sup>9</sup> Because of this brittleness, the development effort has concentrated on two-phase structures containing the hard intermetallic phase  $\text{Cr}_2\text{Nb}$  and the softer Cr-rich solid solution phase. Previous studies indicate that the two-phase Cr- $\text{Cr}_2\text{Nb}$  alloys (CN) exhibited significant plastic deformation prior to fracture under compressive tests at room temperature.<sup>6,7,9</sup> The alloys showed excellent compressive strength at room and elevated temperatures, with the yield strength much superior to nickel-base superalloys and  $\text{Ni}_3\text{Al}$  alloys at and above 1000°C. The CN alloys, however, showed poor fracture strength in tension at ambient temperatures. Because tensile properties were sensitive to defects, efforts aimed at reducing as-cast defects and refining the cast Cr- $\text{Cr}_2\text{Nb}$  eutectic structure led to improved ductility.<sup>10</sup> A room-temperature fracture strength of 548 MPa and an ultimate tensile strength of 388 MPa, and 23% elongation, at 1200°C were achieved, while another CN alloy showed a fracture toughness of 7.6  $\text{MPa}\sqrt{\text{m}}$  at room temperature and 24.4  $\text{MPa}\sqrt{\text{m}}$  at 1000°C.<sup>10</sup>

Current studies are focused on enhancement of fracture resistance in tension at ambient temperatures and oxidation resistance above 1000°C. This report summarizes recent progress on controlling microstructure and improving the mechanical and metallurgical properties and the high-temperature corrosion behavior of Cr- $\text{Cr}_2\text{Nb}$  alloys through alloying additions, material processing, and heat treatment.

## ALLOY PREPARATION AND PROCESSING

CN alloys weighing 430 g were prepared by arc melting and drop casting in a copper mold (2.5 cm diam x 7.6 cm long) preheated to 200°C. High-purity niobium, chromium, and other metal chips were used as charge materials. The cast alloy ingots with the compositions listed in Table 1 generally contained oxide inclusions and cast porosity ranging in size from a few to several hundred microns. The cast alloys also exhibited a coarse eutectic structure with interconnected  $\text{Cr}_2\text{Nb}$  plates, which adversely affect mechanical properties.<sup>8</sup> In order to minimize the cast defects and to refine the eutectic structure, selected alloy ingots were clad inside Mo billets and hot extruded at 1480°C at an extrusion ratio of 4:1. Most alloys were successfully hot extruded into 1.3 cm bar stock.

The CN alloys were also prepared by a powder metallurgy (P/M) route. In this case, elemental powders, in ratios that were chosen to yield the target alloy compositions, were mixed

Table 1. Tensile Properties of Cr-Nb Base Alloys Fabricated by Hot Extrusion at 1480°C

Alloy No.	Alloy Composition (at. %) <sup>a</sup>	Tensile		
		Fracture Strength (MPa)	Yield Strength (MPa)	Elongation (%)
<u>Room Temperature</u>				
CN-80	12Nb-6Mo-1.5Al	548		
CN-90	6Nb-5Mo-4X2-2X3-1.5Al	435		
CN-104	10Nb-6Mo-4X2-0.5X3	293		
CN-112	6Nb-5Mo-2X2-1X3-1X4-1.5Al	508		
CN-113	6Nb-5Mo-2X2-1X3-2X4-1.5Al	374		
<u>1200°C</u>				
CN-80		388	290	23.0
CN-90		384	302	13.4
CN-104		473	371	25.7
CN-112		440	345	30.1
CN-113		414	330	26.4

<sup>a</sup>Balance is Cr.

thoroughly in an inert environment and then placed inside molybdenum cans. The filled cans were then degassed in a vacuum chamber and sealed by electron-beam welding. As above, they were hot extruded at 1480°C to produce CN alloys. All the alloys were successfully hot extruded into bar stock without difficulty.

Within the past year, a series of alloys based on Cr-Cr<sub>2</sub>Zr were also prepared by melting and casting. The advantage of these alloys is that they are more resistant to cast and thermally induced cracking because, unlike the Cr-Cr<sub>2</sub>Nb system, there is a reasonable match between the coefficient of thermal expansion of the second phase and that of the matrix. The alloys with the compositions listed in Table 2 were all successfully fabricated into rod stock by hot extrusion in the same way as the Cr-Cr<sub>2</sub>Nb alloys.

### MICROSTRUCTURAL ANALYSIS

Alloying additions, heat treatment, and material processing all strongly affect the microstructure of the CN alloys. Examination of the microstructure produced by hot extrusion revealed micro-porosity and foreign particles in the P/M products. Energy dispersive x-ray spectroscopic (EDS) analysis indicated that these particles were mainly oxides of aluminum or niobium that formed during materials processing. Apparently, this contamination could not be simply eliminated even though the alloy powders were carefully processed in an inert

Table 2. Tensile Properties of Cr-Zr Base Alloys Fabricated by Hot Extrusion

Alloy No.	Alloy Composition (at. %)	Tensile Fracture Strength (MPa)	Yield Strength (MPa)	Elongation (%)
<u>Room Temperature</u>				
CN-107	Cr-12Zr	304		
CN-114	Cr-8Zr	240		
CN-115	Cr-8Zr-5X1	413		
CN-116	Cr-8Zr-5X1-4X2	443		
CN-117	Cr-8Zr-5X1-4X2-2X3	393		
<u>1200°C</u>				
CN-107				
CN-114		138	108	112
CN-115		267	203	46.3
CN-116		386	281	87.7
CN-117		485	344	28.8

atmosphere. Mechanical tests indicated that the P/M CN alloys had poor fracture resistance at room and elevated temperatures.

Figure 1 shows the optical microstructures of the ingot-processed CN-104 alloy with and without hot extrusion at 1480°C. It, as well as the other alloys listed in Table 1, was given a final heat treatment of 1 d at 1200°C for control of Cr<sub>2</sub>Nb precipitation in the Cr-rich phase. The hot extrusion was effective in breaking up the interconnected coarse Cr<sub>2</sub>Nb phase in the eutectic structure. In fact, it became difficult to distinguish the primary and secondary Cr<sub>2</sub>Nb particles in the alloy after this processing step.

Figure 2 compares the optical microstructures of cast CN-114 and CN-115 fabricated by hot extrusion at 1480°C. Both alloys are based on the Cr-Cr<sub>2</sub>Zr composition containing 8 at. % Zr (see Table 2). Alloy CN-114 is a binary alloy, while CN-115 is a ternary alloy containing 5 % of element X1. The comparison of the microstructures indicates that 5% of X1 is quite effective in breaking up the interconnected Cr<sub>2</sub>Zr phase into blocky particles. All the alloys were also given a final heat treatment of 1 d at 1200°C. It is important to note that, unlike the Cr-Cr<sub>2</sub>Nb system, no precipitation of Cr<sub>2</sub>Zr particles was found in the primary Cr-rich patches. This is consistent with the Cr-Zr phase diagram which shows a very low solubility of Zr in the Cr-rich solid solution phase.<sup>4</sup>

Specimens of the Cr-Nb alloy, CN-90, and the binary Cr-Zr alloy, CN-107, were examined by transmission electron microscopy and energy dispersive spectroscopy (EDS). Both specimens were hot extruded at 1480°C and annealed for 1 d at 1200°C. The matrix of the CN-90 alloy contained a very high density of dislocations while the Cr<sub>2</sub>Nb-based second

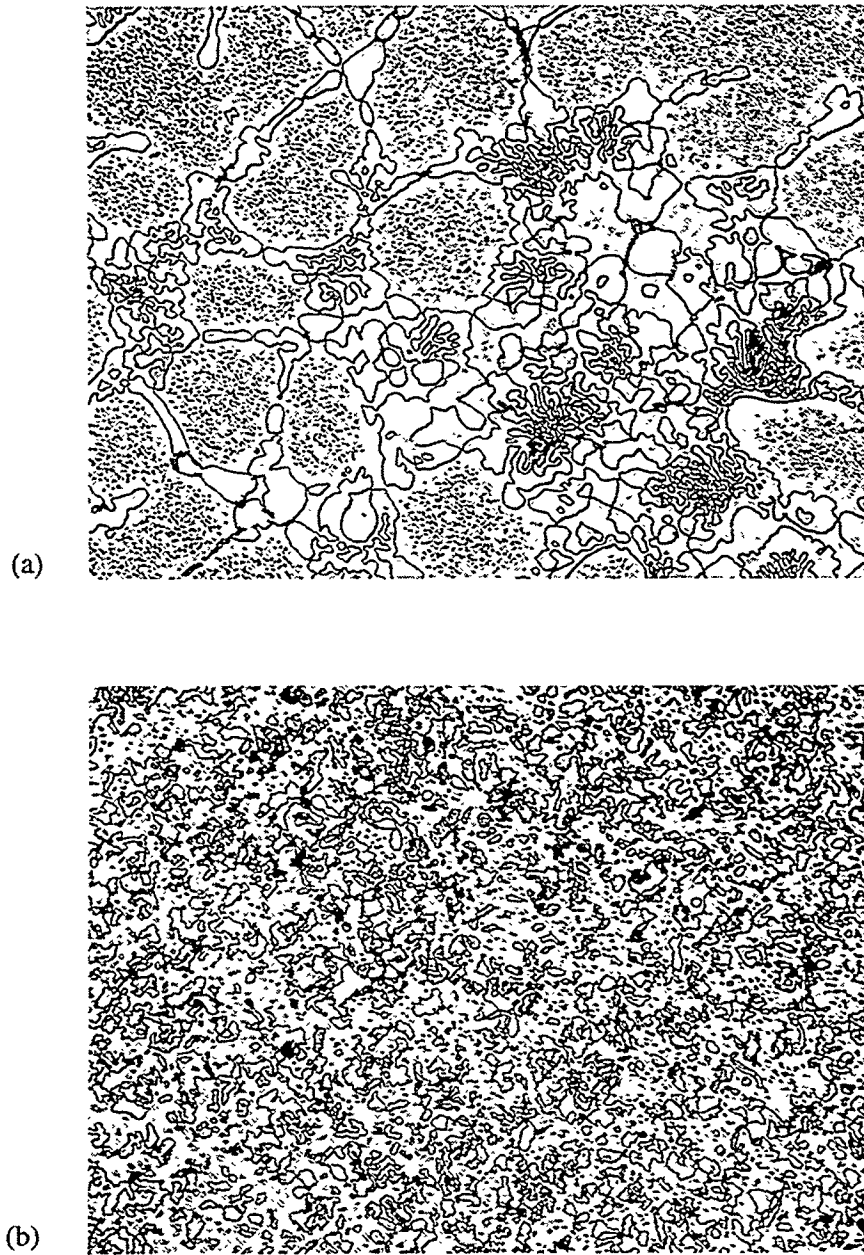


Fig. 1. Optical micrographs of CN-104: (a) as-cast plus annealed for 1 d at 1200°C and (b) hot-extruded at 1480°C plus annealed for 1 d at 1200°C: 625X.

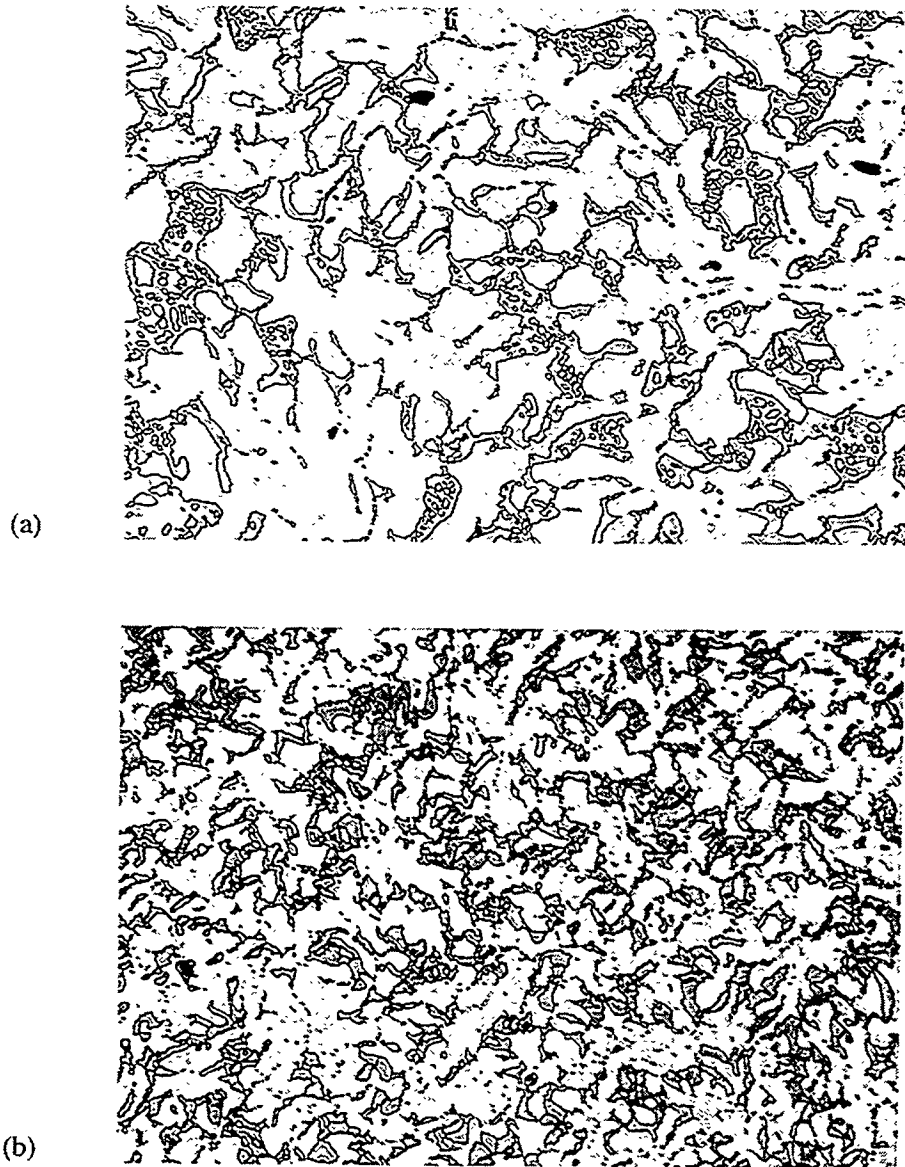


Fig. 2. Micrographs of CN alloys produced by hot extrusion at 1480°C and annealed for 1 d at 1200°C. (a) CN-114 and (b) CN-115; 625X.

phase showed fewer dislocations but some faulting (Fig. 3a). In the CN-107 alloy, (Cr-12% Zr) both the matrix and most of the second phase showed a high density of dislocations even after the 1 d anneal at 1200°C (Fig. 3b). Chemical analyses were performed on very thin areas with the precipitate intersecting the hole and on slightly thicker regions. The analysis of CN-90 showed that the Nb, X2, and X3, elements partitioned strongly to the Cr<sub>2</sub>Nb precipitates, while the molybdenum level in the precipitate matched the matrix. In CN-107, the composition of the precipitate was determined to be 68% Cr - 32% Zr, indicating the expected formation of Cr<sub>2</sub>Zr. Virtually no zirconium remained in solution. Table 3 summarizes the average compositions determined by EDS.

Table 3. Chemical Analysis of CN-90 and CN-107 (in at. %)

CN-90	Al	X2	X3	Cr	Nb	Mo
Average matrix	1	1	1	90	1	6
Average ppt	0.5	11	4	52	25	7
nominal	1.5	4	2	81.5	6	5

CN-107	Cr	Zr
Average matrix	99	1
Average ppt	68	32
nominal	88	12

### TENSILE PROPERTIES

Button-type tensile specimens with gage dimensions 0.31 diam x 0.95 cm long were machined by electro-discharge machining, followed by grinding and polishing with "0" Emery paper. The tensile specimens were tested in an Instron Testing Machine at room temperature in air and at 1200°C in vacuum. Since the tensile properties of brittle materials are sensitive to microstructure and defects in materials, the CN alloys were tested at room temperature for different fabrication conditions. Table 4 compares the tensile properties of CN-90 processed in different ways. The P/M material, fabricated by hot pressing and isothermal forging of the power compact, had the lowest fracture strength, while the material fabricated by hot extrusion of the cast ingot showed the highest value. As mentioned previously, the low fracture strength of the P/M material is associated with interstitial contamination and the formation of oxide/nitride particles.

Table 1 summarizes the tensile properties of Cr-Nb base alloys fabricated by hot extrusion of cast materials. The CN alloys showed no microscopic yielding prior to fracture, and the two alloys CN-80 and -112 exhibited the best room-temperature fracture strength, >500 MPa. At 1200°C, the CN alloys were very strong and ductile. Yield and ultimate tensile



Fig. 3. TEM micrographs of (a) CN 90 and (b) CN 107 showing a high dislocation density present after extrusion at 1480°C and an anneal for 1 d at 1200°C. The  $\text{Cr}_2\text{Nb}$ -based second phase in (a) has few dislocations while the  $\text{Cr}_2\text{Zr}$  second phase in (b) has a higher location density. Bar is 1  $\mu\text{m}$  long.



Table 4. Room-Temperature Tensile Properties of CN-90<sup>a</sup>

Alloy Preparation and Fabrication	Fracture Strength (MPa)
Hot pressing and forging elemental powders at 1480°C	140
Induction melted ingot	169
Hot extrusion of ingot at 1480°C	435

<sup>a</sup>All materials were given a final heat treatment of 1 d at 1200°C.

strengths were above 340 MPa (50 ksi) and 420 MPa (60 ksi), respectively, for both CN-104 and 112. These values are among the highest ever measured for alloys and meet the strength goal of this alloy development program. Alloy CN-112 appeared to have the best combined properties at room temperature and 1200°C. All the alloys except CN-90 had more than 20% elongation at 1200°C.

Table 2 summarizes the tensile properties of the Cr-Zr base alloys fabricated by hot extrusion. Both binary alloys had a low fracture strength, compared to the more highly alloyed compositions. Among all the alloys, CN-116 had the best tensile fracture strength at room temperature. Both yield and ultimate tensile strengths increased substantially with alloying additions, and the alloy CN-117 had the best strength at 1200°C. All the alloys are ductile at 1200°C, with tensile elongation more than 25%. Alloy CN-117 had the best combination of strengths at room temperature and 1200°C.

## HIGH-TEMPERATURE OXIDATION BEHAVIOR

It has been previously demonstrated that the addition of element X2 to Cr-Cr<sub>2</sub>Nb alloys improves oxidation resistance under isothermal and thermal cycling conditions.<sup>10,11</sup> The beneficial influence of X2 was attributed to improvement in the oxidation resistance of the Cr-rich regions (despite its partitioning to the Cr<sub>2</sub>Nb phase),<sup>11</sup> which otherwise showed preferential susceptibility to degradation upon exposure to high-temperature air.<sup>12</sup> However, despite improvements in the oxidation resistance of Cr-Cr<sub>2</sub>Nb alloys, such materials cannot be used in an uncoated condition in oxidizing environments at the very high temperatures where the superior strength of the CN compositions can be exploited (>1100°C). At these temperatures, thermally grown oxides on Cr-Cr<sub>2</sub>Nb alloys are not protective because chromia volatilizes at a significant rate. Oxidation protection will therefore involve the use of coatings. In this regard, silicide coatings applied by a pack cementation process can substantially improve the oxidation

resistance of Cr-Cr<sub>2</sub>Nb alloys.<sup>10,13,14</sup> Such coatings can also protect these alloys against high-temperature sulfidation. As indicated by the data in Fig. 4, which shows specimen weight gain as a function of isothermal exposure time in a highly-reducing H<sub>2</sub>S-H<sub>2</sub>-H<sub>2</sub>O-Ar gas mixture ( $p_{O_2} = 10^{-22}$  atm,  $p_{S_2} = 10^{-6}$ ), a Cr-12% Nb binary alloy was very susceptible to sulfidation, but a Cr-8% Nb composition (CN-87) coated with a Cr-Si layer produced by pack cementation exhibited very low weight gains. The resistance of the coated alloy was comparable to Fe<sub>3</sub>Al alloys containing > 2% Cr, which are considered to have very good sulfidation resistance compared to stainless steels and FeCrAl-type alloys.<sup>15</sup>

Figure 5 compares the isothermal oxidation rate of two more recent Cr-Cr<sub>2</sub>Nb compositions, CN-90 (see Table 1) and CN-100 (8% Nb-6% Mo-4% X2-2% X3), with that of CN-87, which heretofore showed the best oxidation resistance of the CN alloys.<sup>10,11</sup> (Isothermal air oxidation at 950°C has traditionally served as the initial baseline evaluation of oxidation resistance of the CN alloys.) All three compositions shown in Fig. 5 include the same concentration of X2, which, as noted above, has been shown to significantly improve oxidation resistance.<sup>10</sup> Despite this, CN-90 showed a significantly higher oxidation rate. The reason for this is unknown; all of the alloying elements in this alloy are present in comparable concentrations in CN-87 and/or CN-100, which had similar rates of weight gain that were less than that of CN-90. It is possible that the lower Nb concentration of CN-90, and the accompanying distribution of the matrix and eutectic phases, contributes to its higher oxidation rate as such a trend has been established previously,<sup>12</sup> but a definite explanation awaits chemical and microstructural analyses of these specimens. Examination of the data in Fig. 5 and the respective compositions of CN-87, -90, and -100 indicates that iron and element X3 don't have substantial effects on macroscopic oxidation behavior at 950°C.

Alloys based on Cr-Zr will be susceptible to high-temperature oxidation as Zr forms a very stable oxide that grows very rapidly.<sup>16</sup> It is therefore not surprising that the measured weight changes during isothermal oxidation exposures of alloys CN-107 and -114 (Fig. 6) are significantly higher than what is expected for reactions solely controlled by the growth of Cr<sub>2</sub>O<sub>3</sub> (ref. 16) and than what is measured for certain Cr-Cr<sub>2</sub>Nb alloys (Fig. 5). Interestingly, the addition of alloying elements substantially reduced the weight gains and oxidation rate over those measured for the binary compositions - see the results for CN-117 in Fig. 6. There are at least two possible reasons for the observed beneficial effect of alloying. Element X2 may improve oxidation resistance in a similar manner to its effect in the Cr-Nb system.<sup>11</sup> Secondly, as noted above, element X1 effectively breaks up the network of interconnected Cr<sub>2</sub>Zr (Fig. 2). As this phase is much more susceptible to oxidation than the Cr matrix, creation of a finer distribution of Cr<sub>2</sub>Zr may act to reduce the overall oxidation rate. Experiments specifically designed to examine the effects of volume fraction and distribution of Cr<sub>2</sub>Zr, in the context of

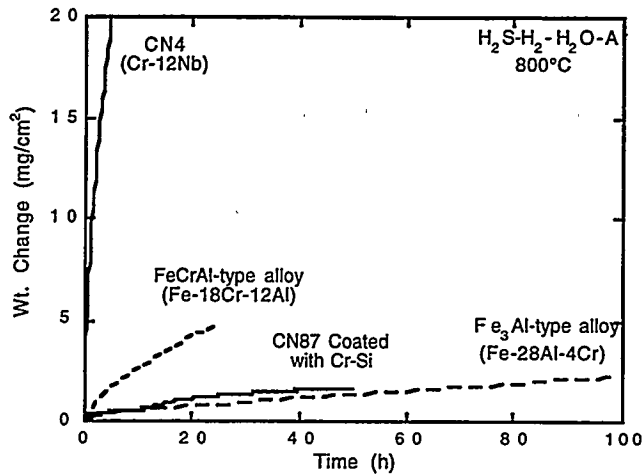


Fig. 4. Weight change as a function of time for alloys isothermally exposed to H<sub>2</sub>S-H<sub>2</sub>-H<sub>2</sub>O-Ar at 950°C. The CN87 alloy consisted of Cr-20%Fe-5%Mo-4%X2-1.5%Al and was coated by a pack cementation process (see ref. 13). Compositions shown are in at. %.

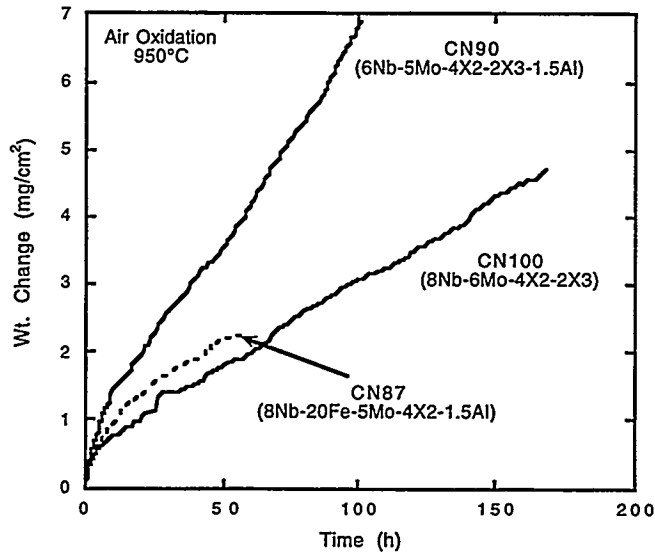


Fig. 5. Weight change as a function of time for Cr-Cr<sub>2</sub>Nb alloys during isothermal exposure to dry air at 950°C. Compositions shown are in at. %.

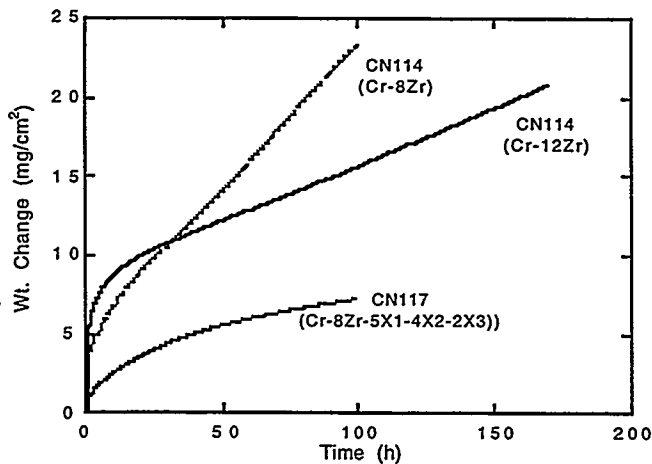


Fig. 6. Weight change as a function of time for Cr-Cr<sub>2</sub>Zr alloys during isothermal exposure to dry air at 950°C. Compositions shown are in at. %.

all the possible processes by which oxide products can grow on two-phase alloys at high temperatures,<sup>17</sup> can best address the validity of this hypothesis.

### FUTURE WORK

The development work on the Cr-Nb system indicates that the alloy CN-112 (Cr-6Nb-5Mo-2X<sub>2</sub>-1X<sub>3</sub>-1X<sub>4</sub>-1.5 Al, at.%) is close to an optimum composition and meets the strength goal of the project. Further studies are required to learn how to scavenge interstitials from the Cr-rich phase in order to achieve good tensile ductility at ambient temperatures. While Cr-Zr alloys show little as-fabricated cracking, there is a need to strengthen the Cr-rich phase by either solid-solution hardening or second-phase precipitation. Oxidation-resistant coatings are needed for the Cr-Zr alloys.

The Cr-rich phase has a limited ductility and fracture resistance at room temperature. In order to significantly improve the room-temperature ductility, the Cr-rich solid solution matrix phase must be substantially modified. Recently, ternary phase diagrams based on the Cr-Nb-X system have been reviewed and new compositions have been identified for alloy development based on a strategy of avoiding as-fabricated cracking and improving the ductility of the matrix in the presence of a Laves phase, which confers the unique high-temperature strength.

### SUMMARY

Alloys of Cr-Cr<sub>2</sub>Nb with exceptionally high strength at 1200°C have been developed. However, these compositions suffer from limited ductility and toughness at room temperature. Despite improvements from processing modifications, as-fabricated defects still limit room temperature mechanical behavior. Alloys based on Cr-Cr<sub>2</sub>Zr show good fabricability because there is only a small mismatch of the coefficients of thermal expansion of the two phases. However, these alloys are generally weaker than Cr-Cr<sub>2</sub>Nb compositions at high temperatures and have poor oxidation resistance. Silicide coatings can provide high-temperature oxidation and sulfidation protection of this alloys. Improvements in room temperature mechanical properties of Laves-phase-strengthened alloys will come from increasing the ductile of the matrix phase by impurity control and compositional modifications.

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STUDY OF FATIGUE AND FRACTURE BEHAVIOR OF NbCr<sub>2</sub>-BASED  
ALLOYS AND INTERMETALLIC MATERIALS: PHASE STABILITY IN  
NbCr<sub>2</sub>-BASED LAVES PHASE ALLOYS

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### ABSTRACT

Phase stability in NbCr<sub>2</sub>-based transition-metal Laves phases is studied in this paper, using data from binary X-Cr, Nb-X, and ternary Nb-Cr-X phase diagrams. It was shown that when the atomic size ratios are kept identical, the average electron concentration factor ( $e/a$  = the average number of electrons per atom outside the closed shells of the component atoms) is the determinate factor in controlling the phase stability of NbCr<sub>2</sub>-based transition-metal Laves phases. The  $e/a$  ratios for different Laves phase structures were determined as follows: with  $e/a < 5.76$ , the C15 structure is stabilized; at an  $e/a$  range of 5.88-7.53, the C14 structure is stabilized; with  $e/a > 7.65$ , the C15 structure was stabilized again. A further increase in the electron concentration factor ( $e/a > 8$ ) leads to the disordering of the alloy. The electron concentration effect on the phase stability of transition-metal A<sub>3</sub>B intermetallic compounds and Mg-based Laves phases is also reviewed and compared with the present observations in transition-metal Laves phases.

### INTRODUCTION

Laves phases are AB<sub>2</sub>-type intermetallic compounds, most of which crystallize in one of the three topologically close-packed structures: cubic C15 — MgCu<sub>2</sub> structure, hexagonal C14 — MgZn<sub>2</sub> structure and dihexagonal C36 — MgNi<sub>2</sub> structure (1). Although Laves phases are in general stabilized by the size-factor principles, that is, the atomic size ratio,  $R_A/R_B$ , is ideally 1.225, with a range of 1.05-1.68 usually observed, the stability of each

crystalline structure is affected by the electron concentration factor. In fact, the electron concentration factor becomes clearly important when the atomic size factors are favorable. The classic work by Laves and Witte (2-3) showed that for several quasi-binary alloy systems involving  $\text{MgCu}_2$  and  $\text{MgZn}_2$ , with increasing valence electron concentration, the three Laves types  $\text{MgCu}_2$ ,  $\text{MgNi}_2$ , and  $\text{MgZn}_2$  exist in that order. For transition-metal Laves phases, average electron concentration was successfully used to correlate the crystal structure by Bardos, Gupta and Beck (4) .

Transition-metal Laves phases have already been in or are being considered for many practical uses, e.g.,  $(\text{Hf,Zr})\text{V}_2$  as superconducting material,  $\text{Zr}(\text{Cr,Fe})_2$  as hydrogen storage material, etc.. More recently,  $\text{HfV}_2$ -,  $\text{HfCr}_2$ - and  $\text{NbCr}_2$ -based two-phase alloys (5-9) are being developed for high-temperature structural uses, because of their good retention of mechanical properties at elevated temperatures. However, their low ductility and brittle fracture characteristics at room temperature are the main concerns for engineering use of these materials.

One attractive way to improve the deformability of complex Laves phases is to control their crystalline structure in the way that stress-assisted phase transformation and/or mechanical twinning can be introduced during plastic deformation (10-11). Thus, it is of uttermost importance to know the factors governing the phase stability in transition-metal Laves phases.

In this study, a number of binary and ternary phase diagrams were surveyed, and the phase stability criteria in the  $\text{NbCr}_2$ -based Laves phase systems X-Cr, Nb-X, and Nb-Cr-X were evaluated. An electron concentration factor ( $e/a$ ) was proposed to control the C14/C36/C15 phase stability in  $\text{NbCr}_2$ -based transition-metal Laves alloys.

#### LAVES PHASE IN BINARY X-Cr AND Nb-X SYSTEMS

Since Laves phases are size compounds, we should choose the X elements in the X-Cr systems with an atomic radius close to Nb and X in the Nb-X systems with an atomic radius close to Cr. In this scheme, we can easily separate the  $e/a$  factor with the atomic size factor in controlling the phase stability. According to this scheme, the X elements selected in the X-Cr system are Ti, Ta, and Nb, and X selected in the Nb-X system are Cr, Mn, Fe, Co, Ni, and Cu. The selection of atom size is based on the consideration of



Goldschmidt radius with 12 coordination numbers (CN) (12). With a minimum disturbance of the atomic size factor, the electron concentration factor,  $e/a$ , should become a dominant one in controlling the phase stability of the binary Laves phases. Here, the  $e/a$  ratio is defined as the average number of electrons per atom outside the closed shells of the component atoms. According to this definition, the  $e/a$  ratio of a transition element is the number of electrons ( $s + d$  electrons) outside its inert gas shells.

Table 1. Atomic Size, Electron Concentration Factor ( $e/a$ ) of Alloying Element, and Existing Binary Laves Phase

Element	Goldschmidt Radii (Å)*	$e/a^+$	$XCr_2/NbX_2$
Nb	1.47	5	$NbCr_2$
Ti	1.45	4	$TiCr_2$
Ta	1.46	5	$TaCr_2$
Cr	1.28	6	$NbCr_2$
Mn	1.31	7	$NbMn_2$
Fe	1.27	8	$NbFe_2$
Co	1.26	9	$NbCo_2$
Ni	1.24	10	None
Cu	1.28	11	None

\* Data from Reference 12.

<sup>+</sup> The unit of  $e/a$  is number of electrons per atom in this paper.

Table 1 lists the Goldschmidt radii (CN=12) and  $e/a$  ratios of all the alloy components, together with the existing Laves phases observed in the binary X-Cr and Nb-X systems. It is interesting to note that Ti and Ta have the atomic radii close to Nb, thus they are postulated to substitute Nb in the  $NbCr_2$  Laves phase. Mn, Fe, Co, Ni and Cu atoms with their atom size close to Cr occupy the Cr positions in the  $NbCr_2$  Laves phase. From the binary X-Cr and Nb-X phase diagrams (13), we can check if the  $XCr_2$  or  $NbX_2$  Laves phase exists in the X-Cr and Nb-X systems, as indicated in Table 1. Also, the mutual solubility, or the homogeneity range of  $XCr_2$  or  $NbX_2$  Laves phase can be read from the binary phase diagrams. Mutual solubility is defined as the difference between the maximum and minimum atomic percents of A in  $AB_2$  phase. Corresponding to the homogeneity ranges, we can simply calculate the  $e/a$  ranges for different binary Laves phases, using the  $e/a$  ratios for various

transition elements listed in Table 1. The binary Laves phase,  $R_A/R_B$  ratio, homogeneity range (%A range), e/a range, and corresponding Laves phase structure are tabulated in Table 2. The Laves structure indicated here is the one stabilized at low temperatures if more than one Laves structure occurring in a binary system. Note that no Laves phases were observed in the Nb-Ni and Nb-Cu binary systems, and that the calculation of phase parameters was based on the imaginary "NbNi<sub>2</sub>" and "NbCu<sub>2</sub>" phases.

Table 2. Atomic Size Ratio ( $R_A/R_B$ ), Homogeneity Range (%A Range), Corresponding e/a Range and Laves Phase Structures in XCr<sub>2</sub> and NbX<sub>2</sub> Alloy Systems

Laves Phase	$R_A/R_B$	%A Range	e/a Range	Structure
TiCr <sub>2</sub>	1.133	35-37	5.26-5.3	C15
TaCr <sub>2</sub>	1.141	33-36	5.64-5.67	C15
NbCr <sub>2</sub>	1.148	30-39	5.61-5.7	C15
NbMn <sub>2</sub>	1.122	25.5-40	6.2-6.49	C14
NbFe <sub>2</sub>	1.157	27-38	6.86-7.19	C14
NbCo <sub>2</sub>	1.167	27-33.3	7.67-7.92	C15
"NbNi <sub>2</sub> "	1.185	33.3	8.34	None
"NbCu <sub>2</sub> "	1.148	33.3	9.0	None

### LAVES PHASE IN Nb-Cr-X TERNARY SYSTEMS

As postulated in the previous section, Ti and Ta occupy the Nb sublattice in NbCr<sub>2</sub> Laves phase. From the Nb-Cr-Ta and Nb-Cr-Ti ternary phase diagrams (14), Ti or Ta substitutes for Nb from 0% to 100% without changing the C15 structure of NbCr<sub>2</sub>. This further confirms our above postulation. For Mn, Fe, Co, Ni, and Cu, they are postulated to substitute for Cr in the NbCr<sub>2</sub> phase. There has no Nb-Cr-Mn ternary phase diagram reported so far, and the Nb-Cr-Cu ternary phase diagrams are incomplete, with the reported data mainly concentrated at the copper-rich corner. On the other hand, the Nb-Cr-Co, Nb-Cr-Fe and Nb-Cr-Ni phase diagrams have been reported in literature (14-15). From these phase diagrams, certain common trends are found: Fe, Co and Ni have certain solubility in the NbCr<sub>2</sub> phase without changing the C15 structure. However, above a certain critical amount

of Co, Ni, or Fe added to NbCr<sub>2</sub>, a phase modification from C15 to C14 is observed. The C14 phase is stable over a wide range of X content. For the Nb-Cr-Co system, a further increase in the Co content results in the reappearance of the C15 structure (15).

Table 3. Homogeneity Range (%X) and Corresponding e/a Range of C15/C14 Structures in Ternary Nb-Cr-X Systems

X	C15		C14		C15	
	%X	e/a	%X	e/a	%X	e/a
Ti	0-33.3	5.33-5.67	--	--	--	--
Ta	0-33.3	5.67	--	--	--	--
Fe	0-4	5.67-5.75	9-66.7	5.85-6.69	--	--
Co	0-3	5.67-5.76	8-62	5.91-7.53	66-68	7.65-7.72
Ni	0-2.5	5.67-5.77	5-52	5.87-8.05	--	--

The stability range of C14/C15 phases in the Nb-Cr-X ternary systems at 1000°C are summarized in Table 3, together with the corresponding e/a values. It should be noted that the solubility of Fe, Co, and Ni in NbCr<sub>2</sub> with the C15 structure decreases in the order of Fe, Co, and Ni. However, the e/a ratios corresponding to the change of the NbCr<sub>2</sub> C15 to C14 structure are almost identical for different systems, implying that an average electron concentration may play a key role in determining the C15/C14 phase stability. Note that the maximum e/a ratio for the C15 structure is about 5.76 and the minimum e/a ratio to stabilize the C14 structure is about 5.88.

### GENERAL DISCUSSIONS

Laves phases are size compounds, therefore, the size difference between A and B atoms is predominant in stabilizing the Laves phase. Since we purposely choose some alloying elements with roughly the same atomic size with either Cr or Nb (see Tables 1 and 2), the size difference between A and B is similar in the AB<sub>2</sub> Laves phases we studied. This approach simplifies our analysis, since we can separate the other factors from the size factor in stabilizing different Laves phase structures. Also, we only choose transition metal to form Laves phase, which makes it ideal to study the e/a effect on the Laves phase stability. In transition metals, filling d-band is

important to affect the phase stability. In Laves and Witte's studies (2-3), Mg-based ternary systems were selected, and a valence electron concentration rule was found to control the occurrence of various Laves structures, with C15 stabilized at low  $e/a$  values, C14 stabilized at high  $e/a$  values, and C36 in between. In their study, both non-transition and transition metals are involved in forming some Laves phases, making it difficult to analyze the valence electron concentration in the alloys, since for transition elements, the valence electron number is not a constant value, varying in different systems.

In the present evaluation, all the elements chosen to form Laves phases are transition metals. Instead of using valence electron concentration, average electron concentration is chosen for correlation purposes. This concept of average electron concentration has been successfully used to obtain a good correlation between the  $e/a$  value and the phase stability in a number of transition metal alloy systems (4, 16-21). If we combine the data in Tables 2 and 3, we can clearly demonstrate the  $e/a$  effect on the phase stability (C14/C15) in NbCr<sub>2</sub>-based Laves alloys, see Fig.1.

At  $e/a$  values lower than 5.76, the C15 structure was stabilized at low temperatures for both binary and ternary Laves alloys. Increasing  $e/a$  to 5.88, the C14 structure was stabilized. Over the  $e/a$  range of 5.88-7.53, the C14 structure is more stable than the C15 structure. This trend is similar to that observed in the Mg-based Laves phases (2-3), where C15 → C36 → C14 phase modification was observed with increasing the  $e/a$  value. However, for the Mg-based Laves phases, this should be considered as a tendency, as it is impossible to classify the compounds in terms of their  $e/a$  ratio. In NbCr<sub>2</sub>-based ternary Laves phases, the  $e/a$  ratio for C15/C14 phase boundaries is very precise, with C15 existing at  $e/a < 5.76$ , and C14 occurring at  $e/a > 5.88$ . This may be associated with the fact, as discussed before, that here all the components of the ternary NbCr<sub>2</sub>-based Laves phases are transition metals. Also, the C36 phase exists between C15 and C14 ranges, with a certain range of homogeneity for the Mg-based Laves alloys. However, no existence of the C36 phase was indicated in the reported phase diagrams of binary and ternary NbCr<sub>2</sub>-based systems, probably due to the difficulty in separating C36 from C14. Both C36 and C14 structures are hexagonal close-packed structures, and many of their X-ray diffraction lines overlap. Considering that C36 may exist between C15 and C14 structures (C36 is a transition structure between C14 and C15, in terms of stacking sequence), it is postulated that in

NbCr<sub>2</sub> based Laves phases C36 may exist in the  $e/a$  regime of 5.76-5.88, probably around 5.7-5.9 due to the possible error in the reported data. In fact, a C36 phase was detected in a recent study of the transition metal Nb-Cr-Fe system (11). Even though it is difficult to calculate the exact  $e/a$  value for the C36 Laves phase since that system is basically a Nb solid solution plus Laves phase two-phase alloy, it does indicate that it is possible to stabilize the C36 structure at certain  $e/a$  ratios.

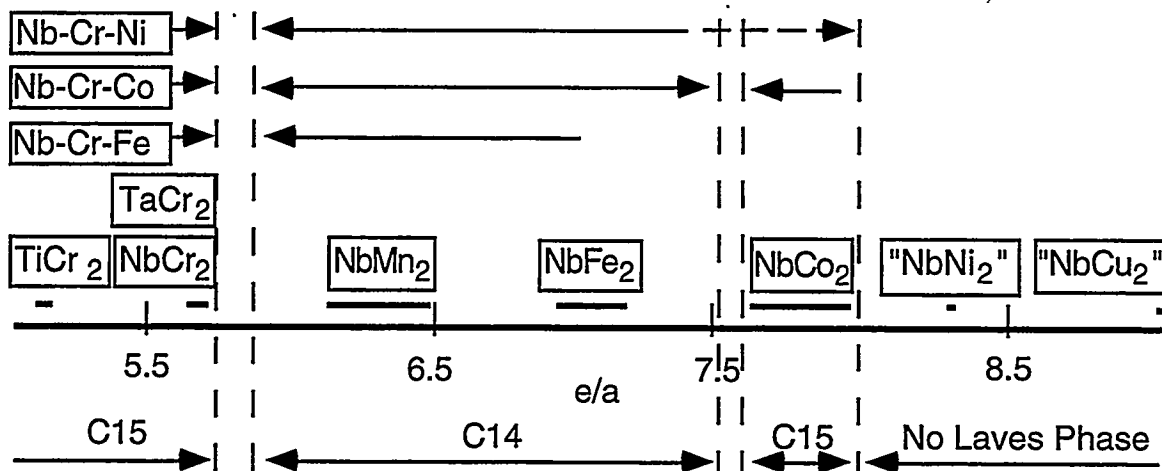


Fig. 1 Effect of electron concentration ( $e/a$ ) on phase stability in NbCr<sub>2</sub>-based binary and ternary systems

The atomic size difference has no effect on the  $e/a$  correlation with the phase stability in both binary and ternary systems. Actually, the solubility of Fe, Co and Ni in NbCr<sub>2</sub> has different values, yet the same critical  $e/a$  value is yielded. These observations may result from the fact that the atomic size difference ( $R_A/R_B$ ) is kept similar in our investigation. However, the size difference may affect the mutual solubility, or homogeneity range of AB<sub>2</sub> Laves phase, as shown in Fig. 2. No good correlation between the  $R_A/R_B$  ratio with the mutual solubility can be inferred from Fig. 2.

The effect of the average electron concentration on phase stability has been shown in many transition-metal A<sub>3</sub>B intermetallic compound systems, usually with a very good correlation obtained (16-18). For example, Liu found that the stacking character of the (Fe, Co, Ni)<sub>3</sub>V ordered alloys can be altered systematically by controlling the  $e/a$  ratio of the alloys (16). Similar to our observation in Laves phase, as  $e/a$  increases, the stacking character changes

from purely cubic to purely hexagonal. However, the critical  $e/a$  ratios for stabilizing the face-centered cubic (f.c.c.) structure ( $< 7.75$ ) and hexagonal close-packed (h.c.p.) structure ( $> 8.54$ ) in  $A_3B$  compounds are different from those for stabilizing the NbCr<sub>2</sub>-based transition-metal Laves phase cubic C15 structure ( $< 5.76$ ) and hexagonal C14 structure ( $> 5.88$ ). The C15/C14

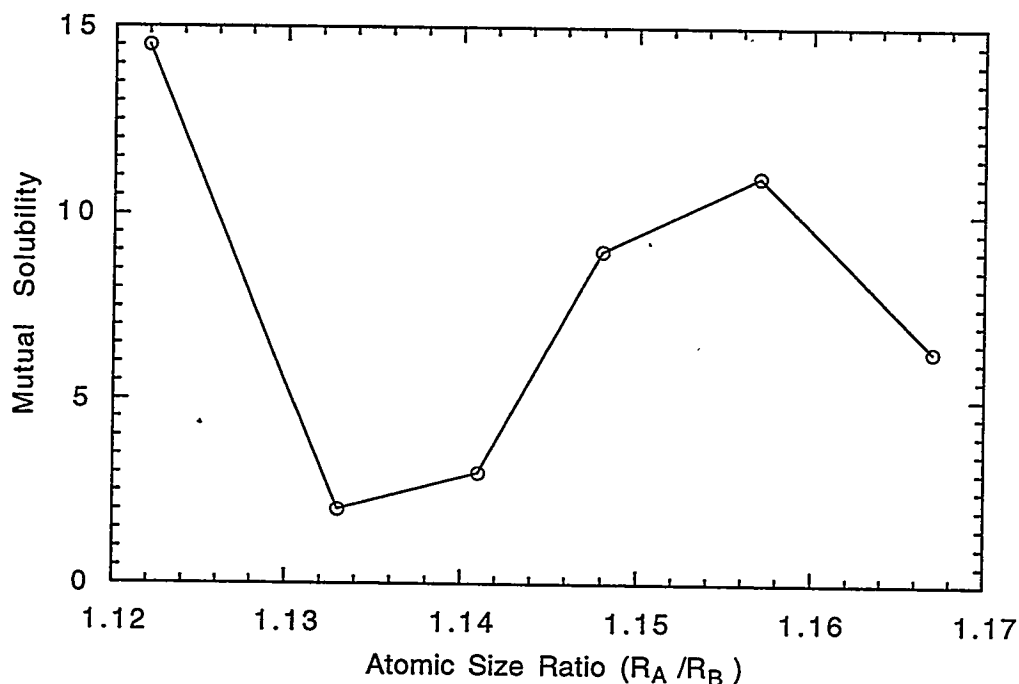


Fig. 2 Effect of  $R_A/R_B$  ratio on the mutual solubility of binary Laves phases

transition in Laves phase systems is sharper than the f.c.c./h.c.p. transition in ordered  $A_3B$  compounds. Also, unlike Laves phase alloys, different ordered mixtures of cubic and hexagonal layers are obtained between the cubic and hexagonal structures for the  $A_3B$  ordered alloys. All the results indicate that the average electron concentration factor has a determinate effect on the phase stability of transition metal intermetallic compounds. The reasons leading to such correlation is not clear now; however, the phase transition in transition metals is known to be related to the filling of an appropriate Brillouin zone.

From Figure 1, we can also see that for the Nb-Cr-Co system, when the  $e/a$  ratio increases further to 7.65, the C15 structure was stabilized again over the C14 structure. This structure modification of C14 to C15 with a further increase in the  $e/a$  ratio has been observed in a number of transition-metal

Laves phases (22). It is a rule, rather than an exception. In ternary Nb-Cr-Mn and Nb-Cr-Fe systems, we can not observe such C14 to C15 transition, since we cannot get  $e/a$  ratio higher than 7.6 in these systems. No NbCu<sub>2</sub> (with  $e/a = 10$ ) and NbNi<sub>2</sub> (with  $e/a = 9.5$ ) Laves phases exist in Cu-Nb and Ni-Nb binary systems, a fact consistent with the observation by Bardos et al. (4) that at  $e/a > 8$ , a disordered structure is stabilized over the Laves phase in transition metal systems. Also in agreement with Bardos et al., the maximum  $e/a$  ratio for the Laves phases in Nb-Cr-Ni system is around 8. However, no C14→C15 transition was reported at  $e/a$  ratio  $> 7.65$ , possibly due to the fact that many ternary phase diagrams containing Laves phases are inaccurate with regard to the identification of C14/C36/C15 structures.

If the electron concentration  $e/a$  correlation with the phase stability is a rule operating in the NbCr<sub>2</sub> based transition-metal alloy systems, it will be possible to modify C15 to C14 and also C14 to C15 by increasingly adding Cu into NbCr<sub>2</sub> to substitute Cr, i.e., by changing the  $e/a$  ratio in the alloy. Systematic work in the direction is being undertaken in our laboratory.

## CONCLUSIONS

Binary X-Cr and Nb-X, and ternary Nb-Cr-X phase diagrams were surveyed, and some interesting phase stability features were identified in these transition metal systems. The average electron concentration factor ( $e/a$ ) has been shown to be a determinate factor in controlling the phase stability of NbCr<sub>2</sub>-based transition-metal Laves alloys. With  $e/a < 5.76$ , the C15 structure is stabilized; at an  $e/a$  range of 5.88-7.53, the C14 structure is stabilized; with  $e/a > 7.65$ , the C15 structure is stabilized again. A further increase in electron concentration ( $e/a > 8$ ) leads to the disordering of the alloy. It is postulated that at  $5.88 > e/a > 5.76$  the C36 structure may be stabilized. The physical background leading to such  $e/a$  correlation with the transition-metal Laves phase stability needs to be further studied.

## ACKNOWLEDGMENTS

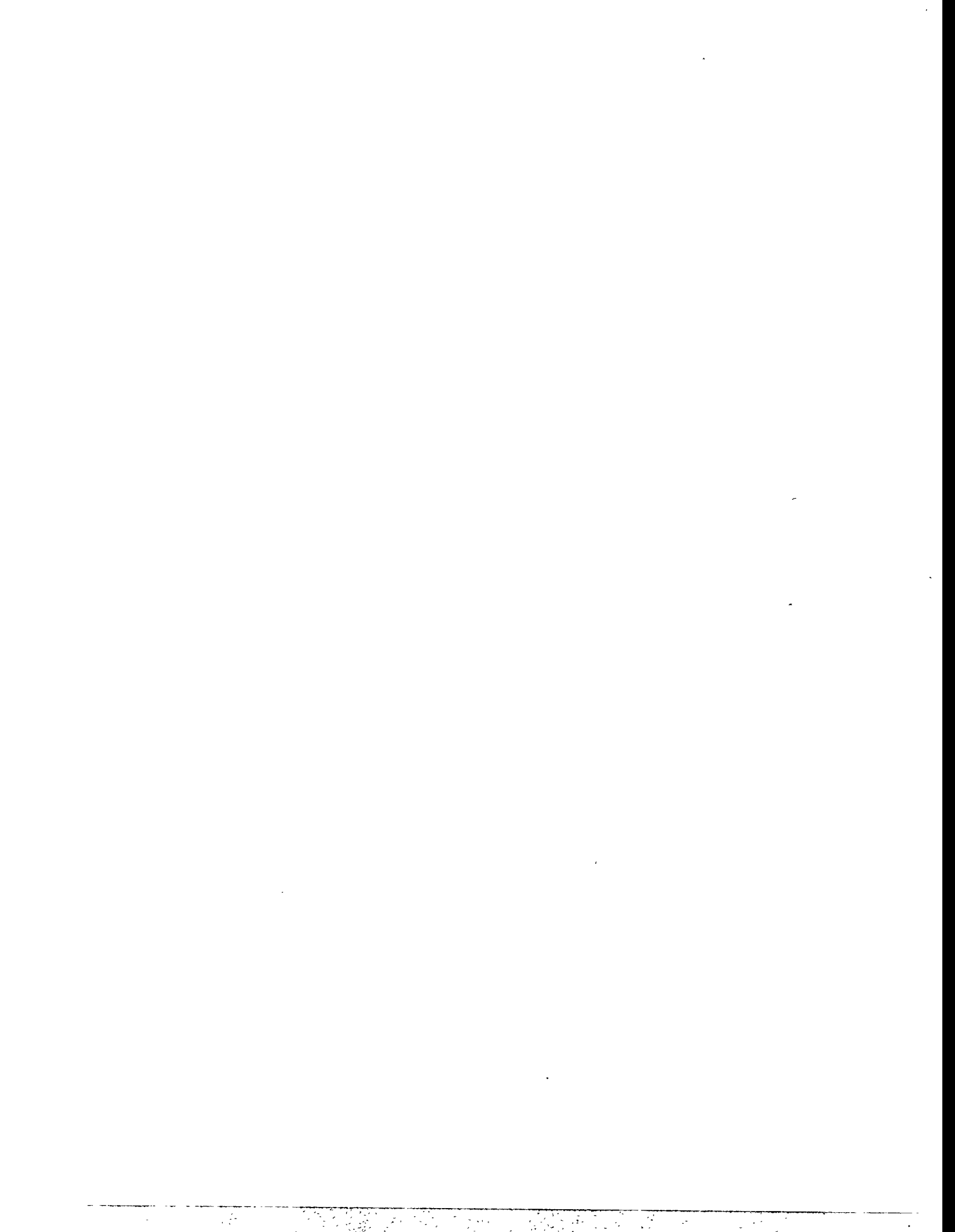
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APPENDIX A  
FINAL PROGRAM



**FINAL PROGRAM**  
**CONFERENCE ON FOSSIL ENERGY MATERIALS**  
**Knoxville, Tennessee**  
**May 14-16, 1996**

**SESSION I - Ceramic Composites and Functional Materials**

**Tuesday, May 14, 1996**

7:00	<b>Registration and Refreshments</b>		
8:00	<i>Welcome and Introductory Remarks, Program Managers, Department of Energy and Oak Ridge National Laboratory</i>	1:00	<i>Corrosion And Its Effect on Mechanical Properties of Materials For Advanced Combustion Systems, K. Natesan, Argonne National Laboratory</i>
8:20	<i>Advanced Research Programs and AR&amp;TD Materials Program Overview - David J. Beecy and James P. Carr, DOE/HQ</i>	1:30	<i>Oxide Coating Development, D. P. Stinton, Oak Ridge National Laboratory</i>
9:00	<i>Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration, T. M. Besmann, Oak Ridge National Laboratory</i>	2:00	<i>Corrosion Protection of SiC Based Ceramics with CVD Mullite Coatings, V. Sarin, Boston University</i>
9:30	<i>Transport Properties of Ceramic Composites, T. L. Starr, Georgia Institute of Technology</i>	2:30	<i>Plasma Deposition of High Temperature Protective Coatings, I. Brown, Lawrence Berkeley National Laboratory</i>
10:00	<b>BREAK</b>	3:00	<b>BREAK</b>
10:20	<i>Joining of SiC Ceramics, B. H. Rabin, Idaho National Engineering Laboratory</i>	3:20	<i>Ceramic Membranes For High Temperature Hydrogen Separation, G. Roettger, Oak Ridge K-25 Site</i>
10:50	<i>Development of Nondestructive Evaluation Methods, W. A. Ellingson, Argonne National Laboratory</i>	3:50	<i>Mixed Oxygen Ion/Electron-Conducting Ceramics for Oxygen Separation, L. R. Pederson, Pacific Northwest Laboratory</i>
11:10	<i>Prediction of Effects of Flaws on Fracture Behavior of Structural Ceramics, J. P. Singh, Argonne National Laboratory</i>	4:20	<i>Preparation and Evaluation of Coal Extracts As Precursors for Carbon and Graphite Products, I. Lewis, UCAR Carbon Company, Inc. and J.W. Zondlo, West Virginia University</i>
11:30	<i>Strength And Corrosion Behavior of SiC - Based Ceramics In Hot Coal Combustion Environments, K. Breder, Oak Ridge National Laboratory</i>	4:50	<i>A Novel Approach to the Removal of Carbon Dioxide, T. D. Burchell, Oak Ridge National Laboratory</i>
12:00	<b>LUNCH</b>	5:20	<b>ADJOURN</b>

**FINAL PROGRAM**  
**CONFERENCE ON FOSSIL ENERGY MATERIALS**  
**Knoxville, Tennessee**  
**May 14-16, 1996**

**SESSION II - Ceramics, New Alloys, and Functional Materials**

**Tuesday, May 14, 1996**  
**6:30 - 8:30 p.m.**

**POSTER PRESENTATIONS - BUFFET RECEPTION**

- |  |  |
|--|--|
| <i>Development of Oxidation-Resistant Composite Materials and Interfaces</i> , D. P. Stinton, Oak Ridge National Laboratory  | <i>Evaluation of Iron Aluminide Weld Overlays for Erosion-Corrosion Resistant Boiler Tube Coatings In Low NO<sub>x</sub> Boilers</i> , J. N. DuPont, Lehigh University |
| <i>Modeling of Fibrous Preforms for CVI Fabrication</i> , T. L. Starr, Georgia Institute of Technology   | <i>Effects of Surface Condition on Aqueous Corrosion and Environmental Embrittlement of Iron Aluminides</i> , R. A. Buchanan, University of Tennessee                  |
| <i>Fiber/Matrix Interfaces for SiC/SiC Composites: Multilayer SiC Coatings and CMZP Oxide Coatings</i> , W. A. Curtin, Virginia Polytechnic Institute and State University | <i>Processing and Properties of Low-Aluminum Alloy FAPY</i> , V. K. Sikka, Oak Ridge National Laboratory   |
| <i>Conditions for Testing the Corrosion Rates of Ceramics in Coal Gasification Systems</i> , J. P. Hurley, University of North Dakota                                      | <i>Microstructural And Mechanical Characterization of Alumina Scales Thermally Developed On Iron Aluminide Alloys</i> , K. Natesan, Argonne National Laboratory        |
| <i>Fracture Behavior of Advanced Ceramic Hot-Gas Filters</i> , J. P. Singh, Argonne National Laboratory  | <i>Overview of the Carbon Products Consortium</i> , C. Irwin, West Virginia University   |
| <i>High Temperature Corrosion of Advanced Ceramic Materials for Hot Gas Filters and Heat Exchangers</i> , C. E. Crossland, Pennsylvania State University                   | <i>Carbon-Fiber Composite Molecular Sieves for Gas Separation</i> , M. Jagtoyen, University of Kentucky  |
| <i>Effect of Heat Treatment at 1150°C on Creep-Rupture Properties of Alloy FA-180</i> , C. G. McKamey, Oak Ridge National Laboratory                                       | <i>Stability of Solid Oxide Fuel Cell Materials</i> , L. R. Pederson, Pacific Northwest Laboratory   |
| <i>The Influence of Composition on Environmental Embrittlement of Iron Aluminides</i> , D. A. Alven, Rensselaer Polytechnic Institute                                      | <i>Proton-Conducting Cerate Ceramics</i> , L. R. Pederson, Pacific Northwest Laboratory  |
| <i>Effects of Titanium and Zirconium on Iron Aluminide Weldments</i> , G. R. Edwards, Colorado School of Mines   | <i>Ceramic Catalyst Materials</i> , A. G. Sault, Sandia National Laboratories  |
|  | <i>Nanoparticle Synthesis in Pulsed Low Temperature Discharges</i> , R. J. Buss, Sandia National Laboratories  |

**SESSION III****WORKSHOP ON MATERIALS RESEARCH AND DEVELOPMENT NEEDS FOR  
THE SUCCESSFUL DEPLOYMENT OF ADVANCED POWER GENERATION  
TECHNOLOGIES****WEDNESDAY, MAY 15, 1996**

Last year's workshop identified several material needs for pressurized fluidized bed combustion (PFBC), integrated coal gasification combined cycle (IGCC), and indirectly fired cycles. This year's workshop will focus on resolution of some of those issues through the definition or redefinition of projects under way.

8:00 a.m. **KEYNOTE ADDRESS: Dr. John Stringer, Executive Scientist,  
Electric Power Research Institute,  
Palo Alto, California**

8:30 a.m. **PLENARY SESSION**

9:00 a.m. **SESSION A. WORKSHOP ON CERAMIC COMPOSITE INTERFACE COATINGS.**

Rapporteurs: R. G. Smith, 3M Company  
R. E. Tressler, Pennsylvania State University  
S. Sambasivan, BIRL  
Moderator: D. P. Stinton, ORNL

Ceramic composites are critical to high-temperature components for fossil energy systems both as hot-gas filters for IGCC and PFBC systems and as structural components, such as heat exchangers, for the indirectly fired cycles, externally fired combined cycle (EFCC), and Combustion 2000 systems. The development of ceramic composites with oxidation resistant interface coatings is extremely important to NASA, the Air Force, and DOE programs. Applications of these composites will be summarized during the workshop and different approaches for oxidation resistant interface coatings will be discussed.

9:00 a.m. **SESSION B. WORKSHOP ON HIGH-TEMPERATURE MATERIALS BASED ON  
LAVES PHASES.**

Rapporteurs: K. S. Kumar, Brown University  
J. H. Perepezko, University of Wisconsin  
D. J. Thoma, Los Alamos National Laboratory  
Moderator: C. T. Liu, ORNL

The Offices of Fossil Energy and Basic Energy Sciences of the Department of Energy are jointly sponsoring this review of critical issues related to alloy development of new high-temperature structural materials based on Laves phases. Laves phase materials, such as the high-temperature Cr-Nb alloys, are of interest because, characteristically, they are high-melting intermetallics that are extremely hard and strong, although brittle. These metallic, rather than ceramic, materials could provide high strengths up to 2300°F for systems such as the IGCC, PFBC, EFCC, and Combustion 2000.

**SESSION III - WORKSHOP (Continued)****9:00 a.m. SESSION C. WORKSHOP ON ALLOYS FOR VERY HIGH-TEMPERATURE APPLICATIONS.**

Rapporteurs: N. Birks, University of Pittsburgh  
 T. B. Gibbons, ABB Combustion Engineering  
 Q. J. Mabbutt, British Gas  
 Moderator: I. G. Wright, ORNL

Systems capable of operating at higher efficiencies, such as the low-emission boiler system (LEBS), require materials with higher temperature capabilities, in particular, higher creep strength and environmental resistance. A range of alloys developed from the best of the currently used wrought ferritic and austenitic alloys have improved high-temperature capabilities, and oxide dispersion-strengthened alloys are targeted for extremely high-temperature applications. This workshop will examine the temperature capabilities of these alloys compared to current alloys and to the needs of advanced systems to identify their appropriate applications, information and actions required or under way to qualify them for such use, and their limitations.

12:00 p.m. **LUNCH**

1:00 p.m. **SESSIONS A & B (Continued)**

**1:00 p.m. SESSION D. WORKSHOP ON MATERIALS ISSUES ASSOCIATED WITH LOW NO<sub>x</sub> COMBUSTION CONDITIONS IN FOSSIL FUEL-FIRED BOILERS.**

Rapporteurs: J. L. Blough, Foster Wheeler  
 J. N. DuPont, LeHigh University  
 S. Kung, Babcock & Wilcox  
 T. B. Gibbons, ABB Combustion Engineering  
 Moderator: I. G. Wright, ORNL

Some cases of severe corrosion of the furnace wall tubes are being experienced in utility boilers fitted with modern, low-NO<sub>x</sub> burners. It has been anticipated for some time that reducing conditions created as part of the low-NO<sub>x</sub> combustion process might result in sulfidation attack, but initial experience with such burners did not reveal such problems. The intent of this workshop is twofold: first, to better define the situation in terms of the form and rate of attack and to examine what is known about its root causes, and second, to review the potential for using corrosion-resistant materials as part of the solution. In particular, if the corrosion is due to sulfidizing conditions, the application of an iron aluminide as an overlay coating may prove a viable option.

3:30 p.m. **WRAP-UP SESSION**

Workshop attendees will gather for summaries of deliberations from Sessions A through D.

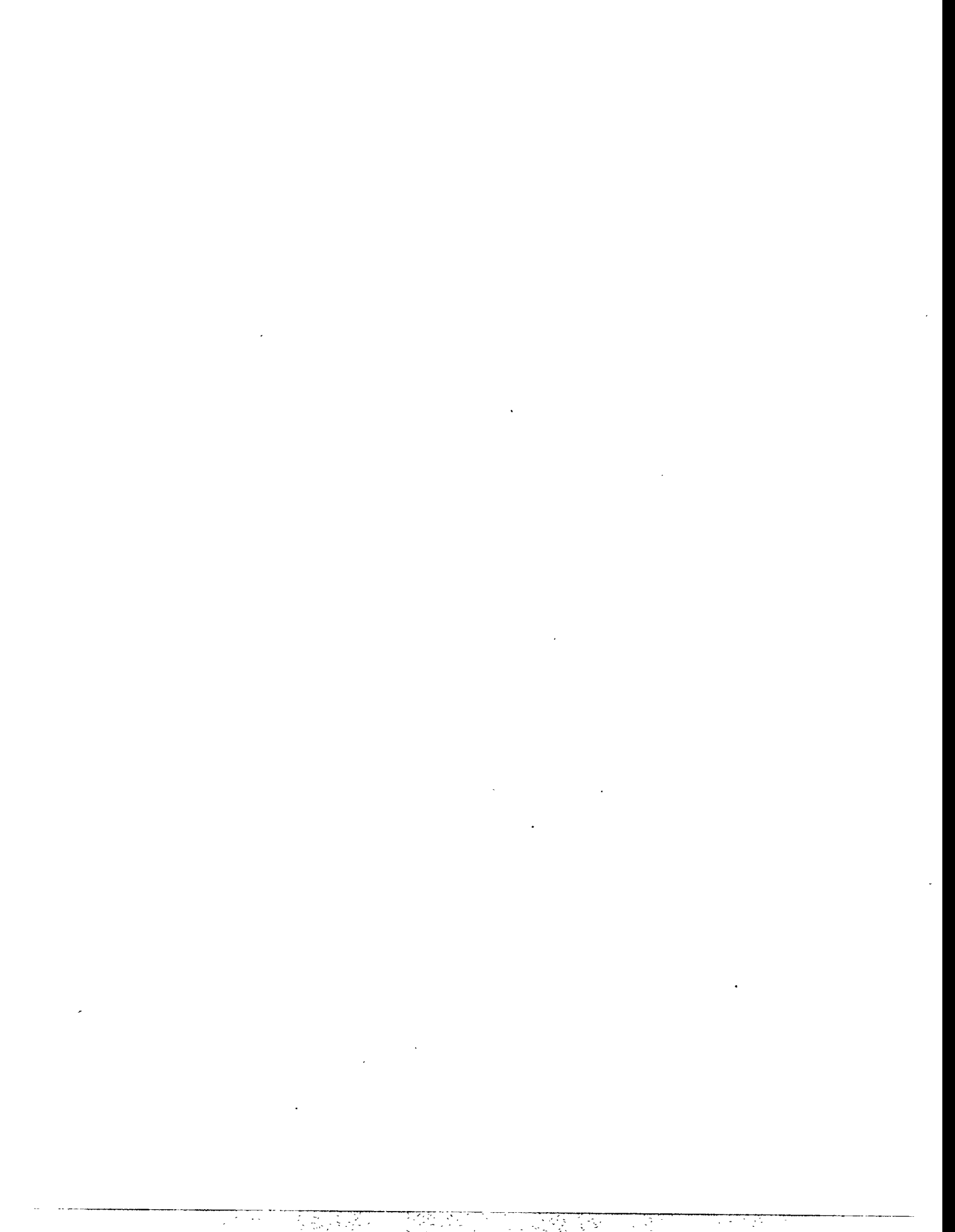
5:00 p.m. **ADJOURN**

**FINAL PROGRAM  
CONFERENCE ON FOSSIL ENERGY MATERIALS  
Knoxville, Tennessee  
May 14-16, 1996**

**SESSION IV - New Alloys**

**Thursday, May 16, 1996**

7:30	<b>Registration Desk Opens</b>		
8:00	<i>Welcome and Introductory Remarks</i>	12:00	<b>LUNCH</b>
8:10	<i>ODS Iron Aluminides</i> , I. G. Wright and E. Ohriner, Oak Ridge National Laboratory	1:00	<i>Investigation of Austenitic Alloys for Advanced Heat Recovery and Hot-Gas Cleanup Systems</i> , R. W. Swindeman, Oak Ridge National Laboratory
8:40	<i>The Influence of Processing on Microstructure and Properties of Fe<sub>3</sub>Al</i> , R. N. Wright, Idaho National Engineering Laboratory	1:30	<i>Microstructural Stability of Base Metal and Weld Metal in 310TaN</i> , C. D. Lundin, University of Tennessee
9:10	<i>Weld Overlay Cladding With Iron Aluminides</i> , G. M. Goodwin, Oak Ridge National Laboratory	2:00	<i>Fireside Corrosion Testing of Candidate Superheater Tube Alloys, Coatings, and Claddings - Phase II</i> , J. L. Blough, Foster Wheeler Development Corporation
9:40	<i>High Temperature Corrosion Behavior of Coatings and ODS Alloys Based on Fe<sub>3</sub>Al</i> , P. F. Tortorelli, Oak Ridge National Laboratory	2:30	<b>BREAK</b>
10:10	<b>BREAK</b>	2:50	<i>Pack Cementation Coatings for Alloys</i> , R. A. Rapp, Ohio State University
10:30	<i>Evaluation of the Intrinsic and Extrinsic Fracture Behavior of Iron Aluminides</i> , B. S. Kang, West Virginia University	3:20	<i>Ultrahigh Temperature Intermetallic Alloys</i> , P. F. Tortorelli, Oak Ridge National Laboratory
11:00	<i>The Mechanical Reliability of Alumina Scales and Coatings</i> , K. B. Alexander, Oak Ridge National Laboratory	3:50	<i>Study of Fatigue and Fracture Behavior of Cr<sub>2</sub>Nb-Based Alloys and Intermetallic Materials</i> , P. Liaw, University of Tennessee
11:30	<i>Electro-Spark Deposition Technology</i> , R. N. Johnson, Pacific Northwest Laboratory	4:20	<b>ADJOURN</b>





**APPENDIX B**  
**LIST OF ATTENDEES**



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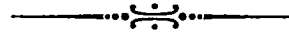
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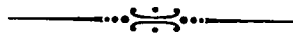
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