

Title: Theoretical and Experimental Investigation on the Low Temperature Properties of the NbCr₂ Laves Phase

Author(s): Dan J. Thoma MST-6, Fuming Chu MST-8
Katherine C. Chen MST-6, Paul G. Kotula MST-CMS
Terence E. Mitchell MST-CMS, John M. Wills T-1
Alim Ormeci, Shao Ping Chen, Robert C. Albers T-11

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Theoretical and Experimental Investigation on the Low Temperature Properties of the NbCr₂ Laves Phase

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Paul G. Kotula, Terence E. Mitchell MST-CMS

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Alim Ormeci, Shao Ping Chen, and Robert C. Albers(T-11)

Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at Los Alamos National Laboratory (LANL). The goal of the project was to develop methodologies in which to define and improve the properties of NbCr₂ so that the high temperature structural applications of alloys based upon this would not be limited by the low-temperature brittle behavior of the intermetallic. We accomplished this task by (1) understanding the defect structure and deformation mechanisms in Laves phases, (2) electronic and geometric contributions to phase stability and alloying behavior, and (3) novel processing of dual phase (Laves/bcc) structures. As a result alloys with properties that in many cases surpass superalloys were developed. For example, we have tailored alloy design strategies and processing routes in a metal alloy to achieve ambient temperature ultimate strengths of 2.35 GPa as well as ultimate strengths of 1.5 GPa at 1000°C. This results in one of the strongest metal alloys that currently exist, while still having deformability at room temperature.

Background and Research Objectives

Applications of Intermetallic Phases

In the past thirty years, intermetallic phases have experienced growing markets in material applications due to their unique properties. For example, the hardness and strength, special magnetic properties, chemical resistance, and semiconducting properties are just a few properties in which intermetallics have found applications. However, the most abundant class of intermetallics, the Laves phases (over 360 defined binary phases), are the least utilized of the intermetallics. Historically, Laves phases have been perceived as a "pest" to the steel and superalloy industries due to grain boundary embrittlement problems associated with the complex structured Laves phase precipitates. For this reason, Laves phases were typically avoided, until it was discovered that Laves phase precipitates,

*Principal Investigator, e-mail: thoma@lanl.gov

distributed in the matrix of ferritic steels (as opposed to grain boundaries), yielded remarkable wear resistant properties. Additional applications of Laves phases, albeit still limited, have been in hydrogen storage, magnetoelastic transducers, and superconductivity.

Recently, intermetallic phases have received considerable attention as structural materials. The high hardness and strength of the materials provide improvements in many engineering applications. In particular, since many intermetallic phases have higher melting temperatures than the respective elemental constituents (due to high heats of formation), high temperature structural applications are particularly engaging (e.g., jet engine applications). A key limitation to the utilization of intermetallics is the low temperature brittleness. Typically, high strength implies strong interatomic bonding, and upon crack initiation, failure is catastrophic. As a result, intermetallics are susceptible to failure before the actual high temperature utilization is achieved.

As with the general historical development of intermetallic phases, Laves phases have lagged in development for high temperature structural applications. The major limitation of Laves phases has been the lack of ductility and toughness in the monolithic intermetallic at low temperatures. However, dual phase alloys of a Laves phase and bcc phase have shown remarkable composite structure toughness. In fact, some recent Laves/bcc phase alloys have been cold-rolled up to 30%. For this reason, over the past five years many companies and institutions in the United States and abroad have started to explore Laves phases for high temperature structural applications. Although dual phase alloys are being pursued, considerable work on the monolithic intermetallic is required to understand and then optimize the mechanical properties.

Laves Phases as High Temperature Structural Materials

Laves phases are ordered intermetallic compounds with the approximate formula AB_2 . The compounds crystallize in primarily one of three crystal structure polytypes: C14 (hexagonal), C15(fcc), and C36(hexagonal). Respectively, the polytypes have 12, 24, and 24 atoms per unit cell, and the structures vary only in the stacking sequence of atom planes (similar to disordered fcc and hcp metals).

The Laves phases are an attractive class of intermetallics for high temperature structural applications. In general, Laves phases retain their high strength (>0.85) at half of the homologous melting temperature, which is the highest of all intermetallics. These phases also have high melting temperatures, excellent creep properties, low densities, and good oxidation resistance.

Among the Laves phases, $NbCr_2$ shows the most promise as a high temperature material. The $NbCr_2$ Laves phase has a melting temperature of 1730°C , appreciable creep resistance, high strength, a density of 7.7g/cm^3 , excellent oxidation resistance below

1100°C, and a relatively large range of binary solubility (up to ~9 atomic percent). In addition, the low temperature phase is the C15 ordered fcc phase (which offers more slip systems than other polytypes), and the congruent intermetallic forms a eutectic with both chromium and niobium solid solutions. The eutectic transformations are an in situ processing methodology to obtain the Laves/bcc dual phase alloys.

Optimization of Low Temperature Properties in the NbCr₂ Laves Phases

To impact the development of the NbCr₂ Laves phases as a high temperature structural material, two material properties need to be improved: ductility and toughness at low temperatures. A complete understanding of the deformation mechanisms and optimal low-temperature mechanical properties for NbCr₂ has not been achieved. Furthermore, the knowledge of electronic structure properties and interatomic bonding is limited. Access to this data through theoretical calculations provides information on the mechanical properties that is difficult to obtain through experiments. These areas were the focus of this study.

The objectives of this project were: (1) to determine completely the mechanical properties, deformation modes, and deformation mechanism of NbCr₂ by high quality processing, mechanical testing, and SEM and TEM characterizations; (2) to understand the electronic structure, interatomic bonding, defect structures, mechanical behavior and deformation mechanisms by the combination of first-principles total energy and electronic structure calculations and atomistic simulations; and (3) to develop alloying schemes in order to optimize the low-temperature mechanical properties of NbCr₂-based alloys.

Importance to LANL's Science and Technology Base and National R&D Needs

Detailed experimental investigations of the mechanical properties of NbCr₂ will more completely characterize the mechanical behavior, deformation modes, and deformation mechanisms in the C15 Laves phase. This will provide a more general understanding for mechanical behavior of Laves phases and similar complex intermetallics. Total energy and electronic structure calculations, in addition to atomistic modeling, will provide information that more completely describes the properties of NbCr₂ and Laves phases in general. With a detailed understanding of NbCr₂, alloying properties can be evaluated to optimize the monolithic intermetallic. In general, a detailed understanding and improvement of the low temperature properties will permit a more generalized application of the abundant Laves phases, which are perceived to be too brittle for many material applications.

Our study of NbCr₂ Laves phases has significant technical impacts. NbCr₂-based alloys have been chosen as potential high-temperature structural materials by a number of institutions in the United States; e.g., Martin Marietta, General Electric, United

Technologies, Southwest Research Institute, NIST, Ladish Corp, and ORNL. In addition, researchers in Germany and Japan are also exploring this material. However, their current efforts are not large.

From a LANL perspective, in addition to energy applications of Laves phases, development of capabilities for alloy design is of primary importance. Such capabilities (both theoretical and experimental) are needed to address alloying phenomena in materials for programmatic needs. Our efforts in this LDRD project have been instrumental in establishing the Alloy Design and Development Team in the Metallurgy Group of the Materials Science and Technology Division at LANL.

Scientific Approach and Accomplishments

Since Laves phases are the largest class of intermetallics, enormous alloying opportunities are available to tailor properties. To target a specific property, effective alloying schemes need to be developed to couple with the desired property response (in this case, deformability). Historically, disordered alloy design strategies were developed through geometric considerations and electronic structure. However, these methodologies are not common for ordered structures, and needed to be elaborated.

The crystal structure for the C15 Laves phase is shown in Figure 1. The unit cell has 24 atoms per unit cell in the nominally AB_2 compound. The A-A and B-B bonding is apparent in the figure, and the like-atom bonding dictates the nearest neighbor bond distances. Using this hardball-type model, geometric rules of size contraction can be developed. For example, the metallic atom size (D) and the intermetallic atom size (d) can be determined from the lattice parameter. The normalized atom size contraction ($S=(D-d)/D$) can be utilized in the relationship for the AB_2 structure S_A+2S_B and can be plotted against the occurrence of solubility in the 360 binary Laves phases, illustrating that solubility occurs when the normalized lattice contraction is between 0-15% (Figure 2). Therefore, binary or ternary alloying requires adherence to this geometric argument [1].

The geometric arguments are a necessary but not sufficient argument for the occurrence of solubility. The electronic structure must be considered. First-principles calculations were utilized to construct density of states determinations. A schematic representation of the Fermi level energy with respect to the density of states for a few early transition element Laves phases are shown in Figure 3. From the extensive work required to calculate this figure, one feature is apparent: rigid band approximations appear to be relevant for interpreting alloying [2-6].

By developing a geometric and electronic basis for interpreting alloying, the final investigation of Laves phases alloying was the interpretation of the substitutional defect

mechanism. A variety of Laves phases were investigated, all leading to the same determination: anti-site occupation is the only observable defect mechanism [7-15].

The property to be tailored, deformability, was investigated with the developed alloying strategies. We determined that deformation in Laves phases occurs by synchroshear. This mechanism requires a cooperative movement of planes of atoms as shown in Figure 4. Deformation occurs in the $\alpha\beta$ stacking sequence. Therefore, to impart deformability to the material, this stacking layer requires substitution of a smaller A atom onto the A sub-lattice. For NbCr_2 , the geometric arguments described earlier only permit titanium, vanadium, or molybdenum as potential alloying elements [1,8,16].

Titanium and vanadium alloy additions to the base NbCr_2 intermetallic were investigated. The experimental ternary diagram construction was required, and isothermal sections are shown in Figure 5. From the experimental investigations, significant ternary solubility could be achieved with both elements. However, titanium appears to substitute for Nb, and V substitutes for Cr. These results were confirmed with ALCHEMI and x-ray diffraction studies. Although expanded phase fields were expected (based upon geometric arguments), the electronic structures defined the subtleties of the alloying behavior. Specifically, the valence contribution of V to NbCr_2 requires a lowering of the Fermi level energy. The Fermi level energy resides on the density of states at a location with partial filling of anti-bonding states, and V substitution for Cr lowers the energy as opposed to substituting for Nb. Similar arguments can be used for Ti substitution onto Nb sites [8,11,14,15].

Based upon the arguments presented, Ti should be the alloy addition that enhances deformability in NbCr_2 . Hardness indentations tests were used to test the hypotheses. The hardnesses for the $\text{Nb}(\text{Cr},\text{V})_2$ alloys are shown as a function of temperature in Figure 6. The brittle to ductile transition temperature increases with increasing vanadium content, illustrating that the V additions decrease the deformability of the monolithic phase. This is consistent with a larger B atom substituting for the Cr atom, therefore locking the synchroshear mechanism. However, the hardness and toughness of $(\text{Nb},\text{Ti})\text{Cr}_2$ illustrates a reverse trend (Figure 7). With the smaller Ti substituting for Nb, synchroshear is less constrained, and the toughness increases with Ti additions [8,16].

Since alloying strategies were developed and coupled with determination of the methodology for deformability, the final aspect of achieving a viable engineering alloy was designing a dual phase alloy. Despite improvements in the deformability of the monolithic intermetallic, the material was still too brittle for, as an example, a turbine blade. Therefore, based upon the Nb-Cr-Ti phase diagram, an alloy with maximum solubility in the Laves phase within a refractory bcc matrix was processed. The alloy composition was

Nb-37at%Cr-27at%Ti. Initially, a 3-kg ingot was cast in a plasma-arc melting (PAM) technique. X-ray work suggested that 15 vol% of the Laves phase was suppressed, but the intermetallic resided at the grain boundaries, thus limiting the full strength of the material. Therefore, 250-gram ingots were rapidly solidified into a ribbon form using chill-block melt spinning. The product was pulverized and consolidated through hot isostatic pressing (HIP) [17-19].

The materials were tested in compression under quasi-static conditions as a function of temperature, and the results of the two processing techniques are shown in Figure 8. Room temperature yield strength and ultimate flow stress for the as-cast alloy are 1620 and 1800 MPa, respectively, and for the HIP alloy, 1680 and 2350 MPa. The as-cast alloys show 16% plastic strain, while the HIP alloy demonstrate less than 2%. Microstructural differences between the PAM and HIP alloys cause different fracture modes and deformation mechanisms. Microcracking within the Laves phase was observed for the as-cast alloy, while interface cracking occurs in the HIP alloy. Intergranular fracture was also found in the HIP alloys. Both alloys showed significant plasticity in compression at 1200°C, and have strengths greater than 70 MPa. No cracking occurs, and dislocations are found in the Laves phase [17-19].

The most important accomplishment of this effort was development of a viable alloy with significant strength up to 1200°C, which is higher than any superalloy. The strengths at room temperature are one of the highest values of any metallic system ever discovered. As a result, we surpassed all project goals from an engineering perspective.

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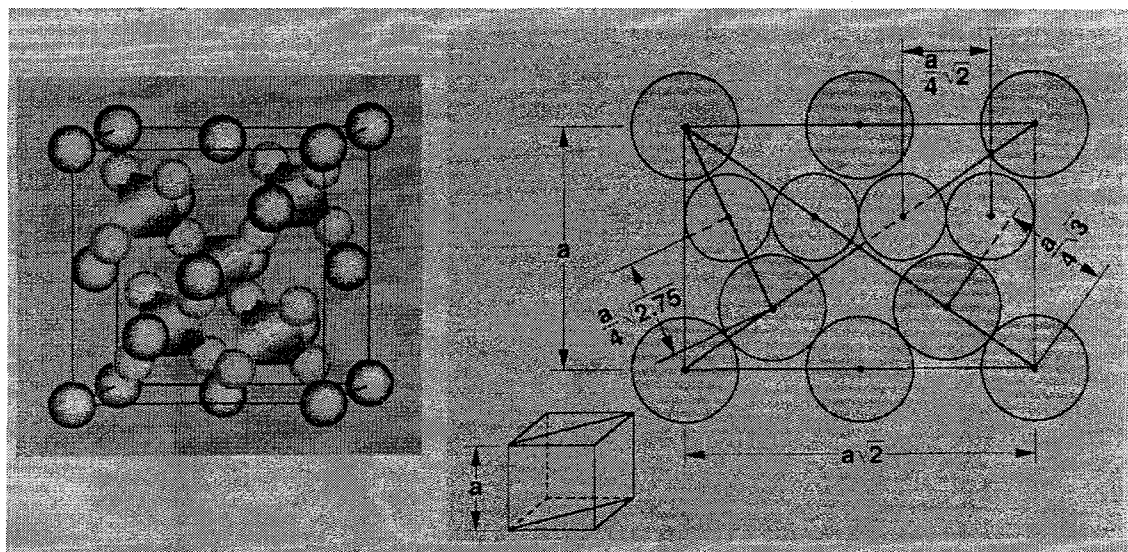


Figure 1: C15 Laves phase crystal structure.

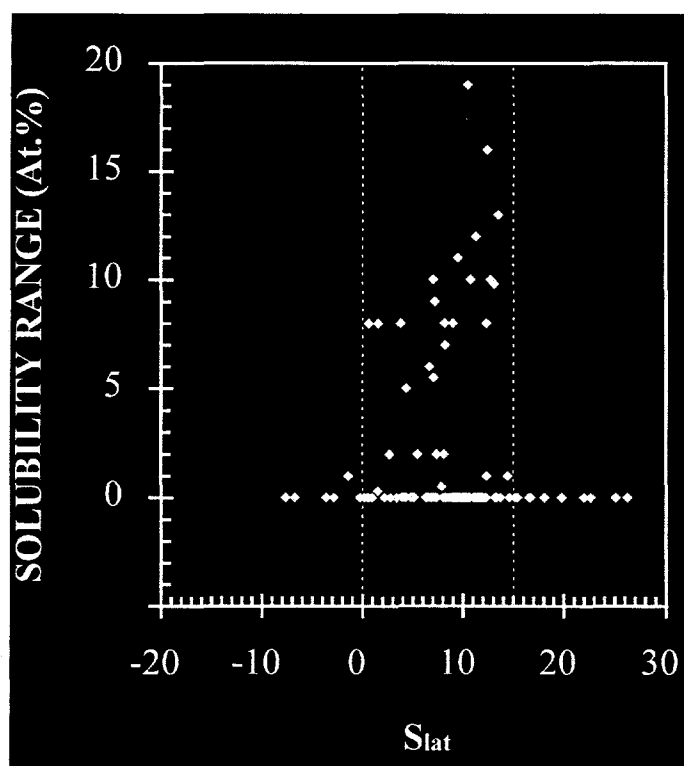


Figure 2: Solubility in Laves phases as a function of the normalized lattice adjusted contraction

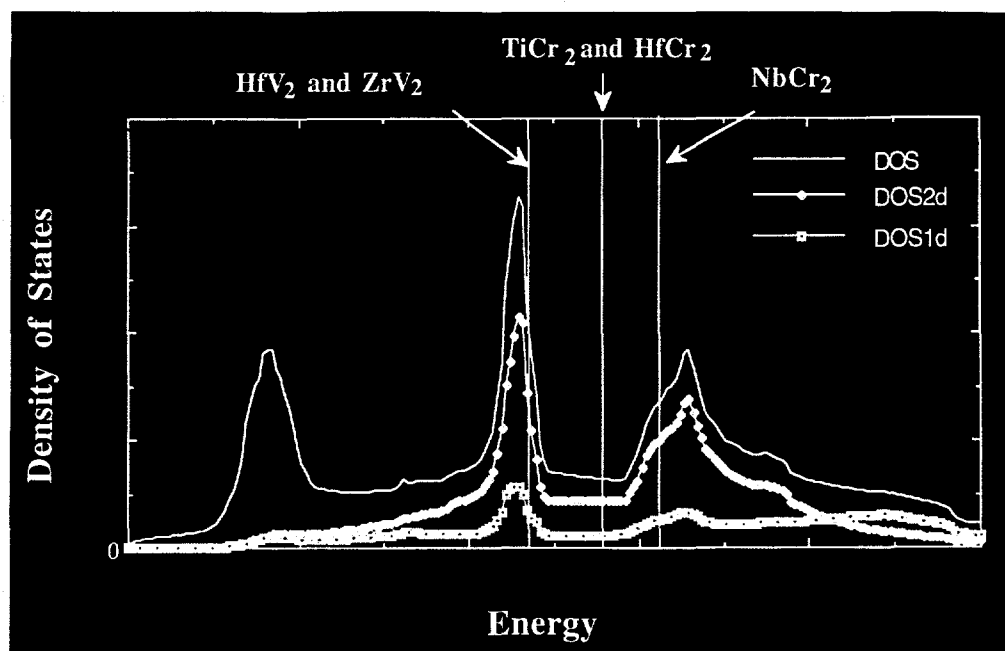


Figure 3: Density of states schematic for early transition metal C15 Laves phases.

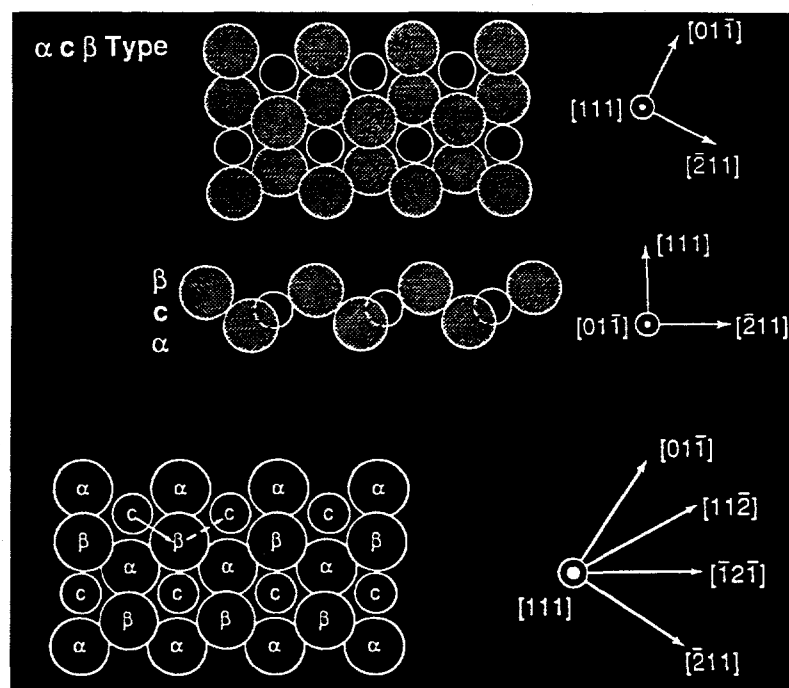


Figure 4: Schematic illustration of synchroshear in Laves phases.

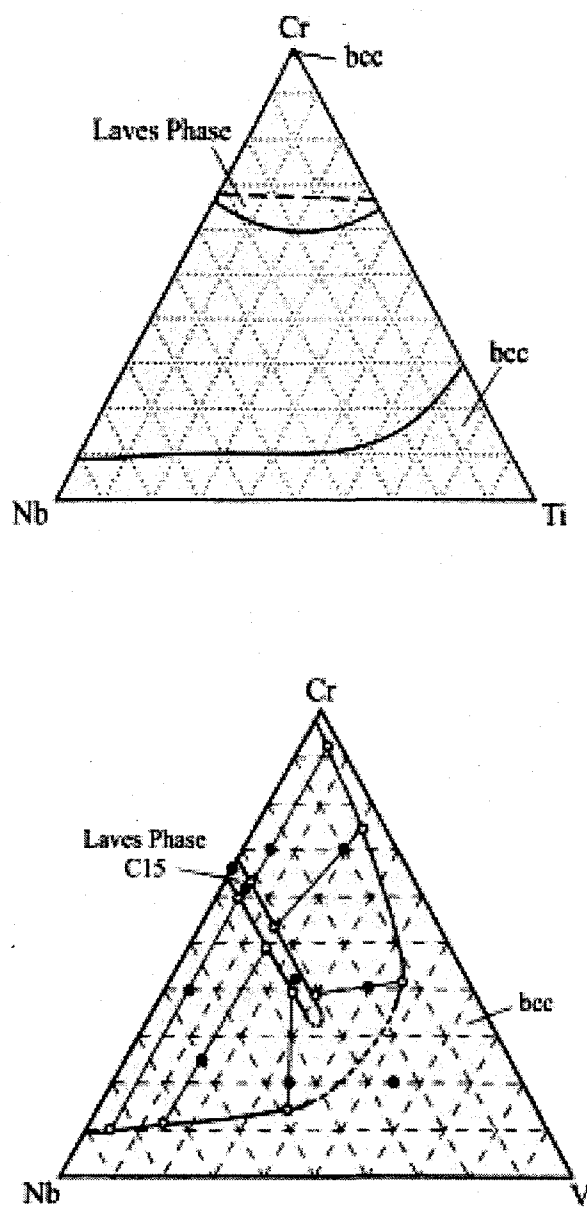


Figure 5: Ternary phase diagrams (Nb-Cr-X, X=V,Ti).

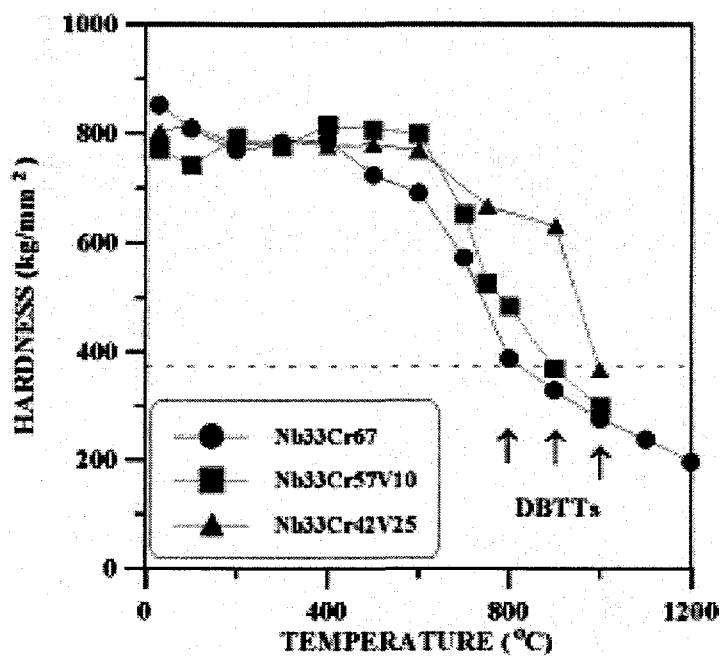


Figure 6: Hot hardness indentation testing of Nb(Cr,V)₂, illustrating an increase in the brittle to ductile transition temperature (DBTT) as a function of increasing vanadium content.

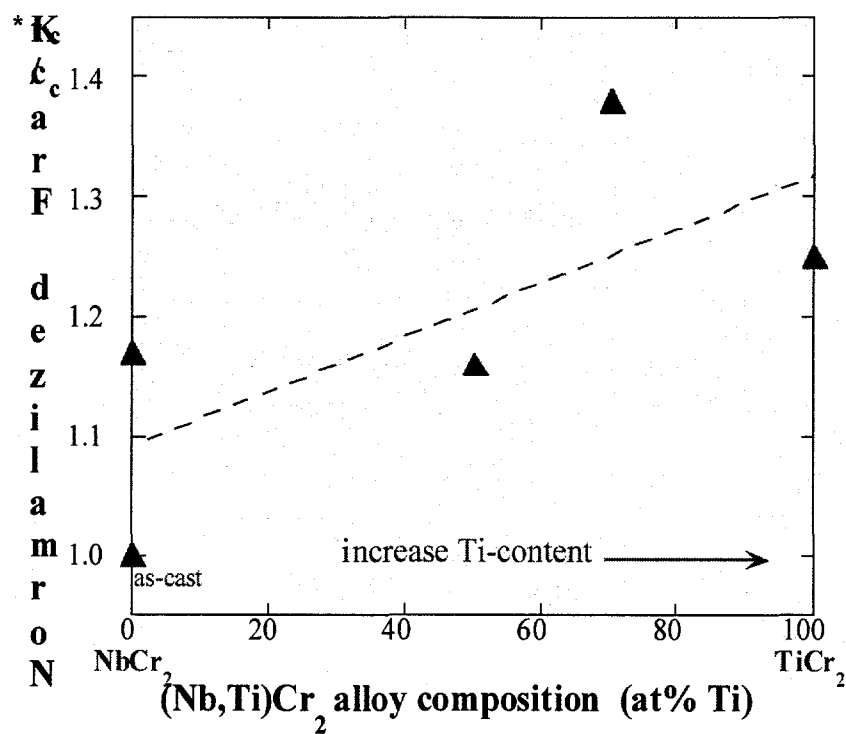
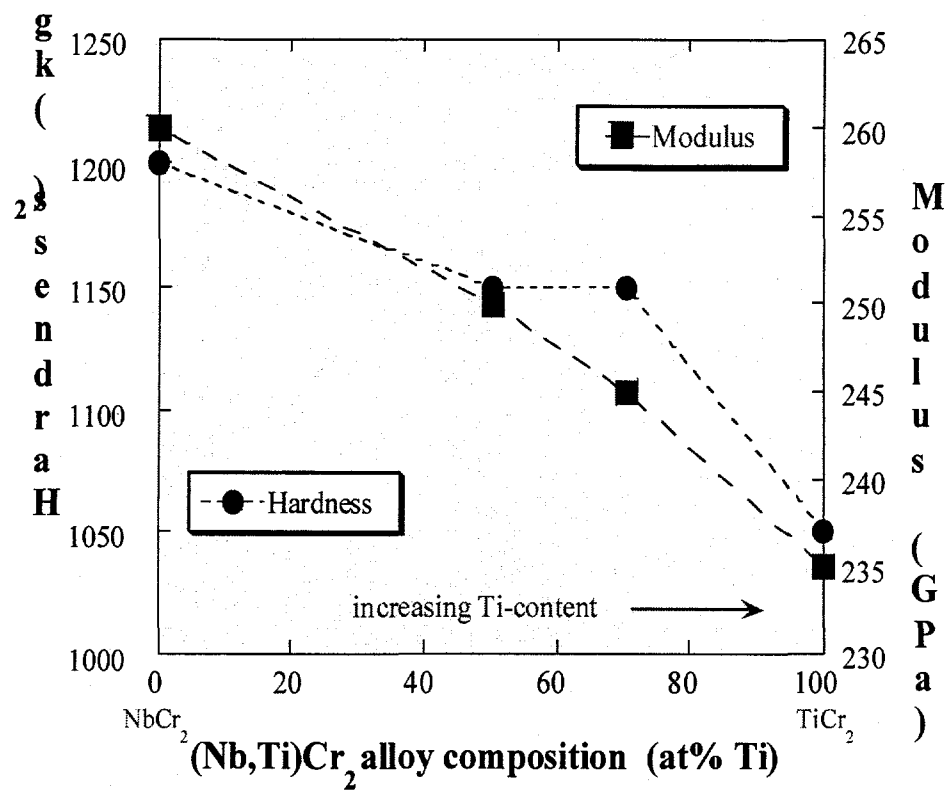


Figure 7: Indentation properties of (Nb,Ti)Cr₂.

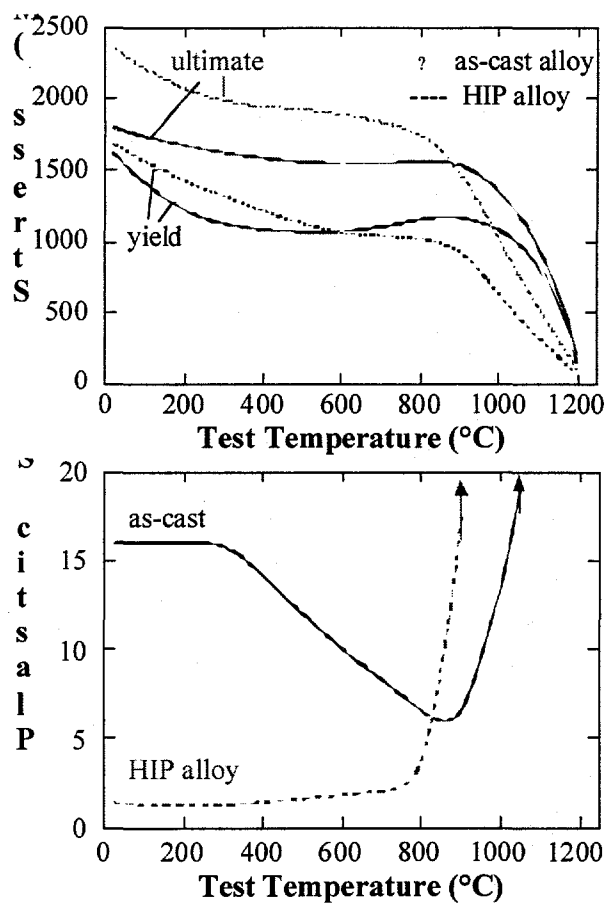


Figure 8: Yield and ultimate stress (top panel) and plastic strain (bottom panel) as a function of compression test temperature of the as-cast (bold lines) and the HIP alloy (dashed lines).