High pressure investigation of ductile intermetallic HoCu

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Abstract  The results of high-pressure angle dispersive X-ray diffraction measurements up to 27.8 GPa on the ductile intermetallic HoCu is presented. The ambient CsCl structure \((SG: Pm\-3m)\) is found to be stable upto the highest pressure of the present measurements. The pressure-volume data fitted to second order Birch-Murnaghan equation of state yields the bulk modulus and its pressure derivative as 76.8 GPa and 4 respectively.

1. Introduction
Intermetallic compounds have always attracted considerable attention as an engineering material due to their interesting combination of mechanical, electrical, magnetic, thermal and elastic properties that are often superior to ordinary alloys. Many of them possess desirable combinations of low density, good oxidation resistance and high strength at elevated temperature. However, their engineering application has been limited by the generally poor ductility and low fracture toughness and brittle behaviour at ambient temperature [1]. Recently however a large family of fully ordered stoichiometric binary rare earth intermetallic compounds with high ductility and high fracture toughness at room temperature have been reported [2]. Combining a rare earth element “R” (Y, Dy, Ho, Er, Ce, and Nd) with metals “M” like Cu and Ag forms these equiatomic binary compounds “RM” with CsCl type structure \((SG: Pm\-3m)\) as shown in Figure 1 wherein the corners of the unit cell cube are occupied by the “M” element and the atom in the cube centre is the “R” element. These RM compounds are “line-compounds” with the exact 1:1 stoichiometry. These ductile materials are promising materials for coatings that are highly resistant to corrosion or that maintain strength at high temperature. Many theoretical and experimental investigations have been carried out to reveal the mechanism of the high room temperature ductility in these RM intermetallics because it may provide insights into improving ductility in other intermetallics [3-6].

A number of features make the observation of ductility even more striking. Calculations by Morris et al [3] have shown that the RM ductile materials are significantly different than previously studied intermetallic B2 compounds. The elastic constants are significantly more isotropic, and the Poisson’s ratio is smaller. The bonding in these materials is less covalent than, for example, NiAl, which shows significant ductility only in single crystals oriented for single slip modes. The fracture toughness value for the RM compounds is two to five times larger than that of NiAl (which also has the B2 structure) but about the same as that of aluminium alloys. Also, the tensile strength and elongation values for the RM phases and commercial grade aluminium alloys are comparable, but the elongations are five to ten times larger than that of the brittle NiAl intermetallic compound [4]. The high fracture toughness
observed in these RM compounds has been attributed to their multiple slip systems, fine grain size and to the possible “R” element counteracting environmental embrittlement [5]. Gschneidner et al [1] have indicated that these materials possess much lower unstable stacking fault energies due to which it is easier for them to plastically deform instead of fracturing at the grain boundaries. Furthermore theoretical calculations have indicated the Fermi energy to be near a local minimum for some of the RM systems and the hybridization in these systems has been found to be stronger than that of NiAl alloy indicating a better ductility in these intermetallics than the NiAl alloy [6].

![Figure 1. Crystal Structure of HoCu.](image)

HoCu belongs to this class of ductile intermetallics. Neutron diffraction [7] studies on a related compound GdCu have indicated a diffusionless martensitic transformation from the ambient CsCl to orthorhombic FeB structure over a broad temperature range near the Neel temperature. This phase transition is characterized by pronounced anomalies in unit cell volume and electrical resistivity. Heat capacity [8] and thermal expansion [9] measurements on HoCu and DyCu have indicated anomaly near 26 K and 61K respectively. These low temperature anomalies are related to spin reorientations and antiferromagnetic transition [10]. The structural instability in this series of compounds have been correlated with the magnitude of the metallic radii of the rare earth ion, which produces small variation in the density of states near the Fermi level [9]. To get a better understanding of the anomalous ductility of RM intermetallics, fundamental investigations of their structural properties are desirable. Application of intensive variables e.g., pressure, is known to influence the structure and properties of materials. The present synchrotron based high pressure angle dispersive X-ray diffraction (ADXRD) on HoCu up to 27.8 GPa is aimed at investigating its structural stability under compression.

2. Experimental Details

HoCu was prepared from pure metal constituents by argon arc-melting in a water-cooled copper hearth. The sample characterization using XRD indicated a cubic symmetry (SG: Pm 3m) with a lattice parameter of 3.440 Å. High pressure ADXRD measurements were carried out on powdered HoCu at the synchrotron radiation source at Elettra, Trieste, Italy. A Mao-Bell type diamond anvil cell (DAC) with diamonds of culet size 400 μm was employed. Fine powder of HoCu along with silver as the internal pressure calibrant was loaded into a hardened stainless steel gasket of hole 150 μm in diameter with 4:1 methanol:ethanol as the pressure-transmitting medium. The experimental station was based on an image plate area detector (Marresearch). The sample to image plate distance and wavelength were calibrated using LaB₆ as standard. The X-ray beam wavelength was calibrated to be 0.652 Å. The data was collected up to a pressure of 27.8 GPa with a typical exposure time of about 200 secs depending on the beam current. The scanned two-dimensional diffraction patterns were corrected for image plate tilt and converted to intensity vs 2θ through radial integration using FIT2D.
The lattice parameters of the sample and silver were determined by carrying out full profile refinement using GSAS software [12]. The pressure was then determined from the equation of state of silver [13].

3. Results and Discussion

The evolution of the diffraction pattern at various pressures as seen in Figure 2 shows that the ambient cubic phase is retained up to the highest pressure of 27.8 GPa attained in the present measurements. There was no indication of any pressure-induced phase transition in the investigated pressure range.

![Figure 2. Evolution of ADXRD pattern with Pressure for HoCu](image)

The pressure volume (P-V) data obtained at various pressures is shown in Figure 3. A second order Birch-Murnaghan equation of state fit to the pressure volume (P-V) data yielded a bulk modulus of 76.8 GPa with its pressure derivative fixed at 4.

![Figure 3. Equation of state for HoCu](image)
The results of the present investigation are also consistent with the recent study on the deformation behavior of DyCu ductile intermetallic compound under compression which showed no indications that DyCu had undergone stress-induced phase transformation or twinning [14].

4. Conclusions
The ductile intermetallic HoCu has been investigated by high-pressure synchrotron powder diffraction for its structural stability up to 27.8 GPa. A second order Birch-Murnaghan equation of state fit to the pressure volume (P-V) data yielded a bulk modulus of 76.8 GPa with its pressure derivative fixed at 4.

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