

Synchrotron Infrared Spectroscopy of BC₂N

Z. Liu (CIW), R. Hemley (CIW), Y. Zhao (LANL), D. He (LANL) and J. Zhang (SUNY)
Beamline(s): U2A

Introduction: Superhard nanocrystallites embedded in a strong amorphous matrix is currently the most promising concept for the synthesis of novel superhard material in bulk form. It is known that the achievable strength and hardness of engineering materials are usually orders-of-magnitude lower than the theoretical values. The reason for this is that deformation and fracture occur through the multiplication and propagation of vacancies and dislocations in crystalline materials. The initiation and growth of microcracks in grain boundaries of ceramics and metal alloys lead to significantly lower practical hardness, toughness, and strength than the theoretical values. Nanocrystalline and amorphous phases greatly minimize these drawbacks and enhance their mechanical performance substantially. The amorphous boundary has significant advantages over the crystalline boundary, including: 1) relaxing mismatches from adjacent unit cells corresponding to different phases; 2) absorbing vacancies, dislocations, and impurities at boundaries; and 3) diminishing surface energy and reducing residual stresses among the nanocrystalline grains. The amorphous boundaries, therefore, substantially improve the stability and mechanical performance of nanostructured bulk materials. In this work, we use synchrotron infrared (IR) technique to characterize the synthesized B-C-N superhard ternary phase and try to confirm the existence of the ternary BC₂N single phase based on the changes of vibrational spectra between starting materials and the synthesized composites.

Methods and Materials: The materials studied are diamond+cBN mixture and BC₂N synthesized at 20 GPa and 2200 K. The IR microspectroscopic studies on these samples were conducted using a synchrotron radiation source (U2A at NSLS). The samples were squeezed into thin films of about one micrometer thickness using diamond anvils. The IR absorption measurements were carried out on the diamond anvil or a KBr substrate.

Results: There are three features in the observed synchrotron IR spectra as shown in Fig. 1: 1) the diamond absorption band at 1280 cm⁻¹ vanishes for the BC₂N sample on the KBr substrate; 2) the B-N bonding band from cBN at 1100 cm⁻¹ shifted to 1085 cm⁻¹ in the BC₂N phase; 3) all diamond absorption bands between 1900 and 2300 cm⁻¹ disappeared totally for the BC₂N sample measured on the KBr substrate. More importantly, the synchrotron IR absorption spectra show clear new peaks for the BC₂N sample at 892, 1442, and 3233 cm⁻¹, which correspond to neither diamond nor cBN. The appearance of these new vibrational modes reflects the different bonding and the greater complexity of the BC₂N crystal structure. The new modes are presumably C-N and B-C vibrational modes. This synchrotron IR absorption spectroscopic study provides evidence for the existence of the ternary BC₂N single phase. It is noteworthy that only the squeezed thin-film BC₂N samples can be removed from the diamond anvil in one piece and placed on the KBr substrate for IR experiments. The thin films of the diamond-cBN samples do not stick together well and thus cannot be transferred from the diamond anvil to the KBr substrate. It is also extremely noteworthy that the color of our BC₂N sample is translucent yellowish at mm-thickness, becoming transparent with light yellow color at micrometer thickness. This is in contrast to the dark color of the synthesized diamond + cBN at any thickness.

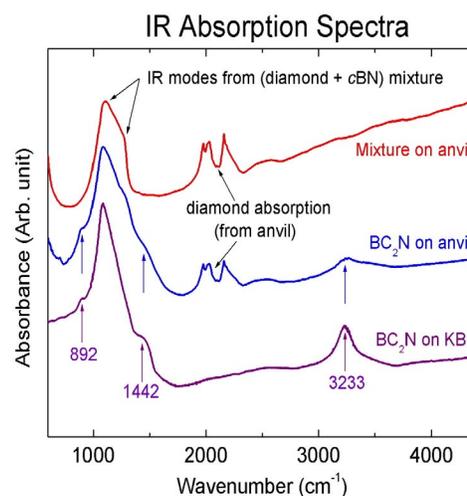


Fig. 1. Synchrotron IR absorption spectra of the diamond+cBN composite (top) and the BC₂N phase on a diamond anvil (mid) and on a KBr substrate (bottom). The disappearance of diamond absorption bands and shifting of the B-N bands and, more significantly, the appearance of new bands in the BC₂N spectrum illustrate the existence of new bonding structures in the single BC₂N ternary phase.