

Title: Innovative synthesis at high pressure and temperature of icosahedral ternary phases B_xCSi_y with improved mechanical properties

Keywords: hard material, boron carbide, HPHT synthesis

Scientific description:

Boron carbide is a ceramic of utmost importance for both its mechanical and nuclear properties. It has been selected as the (only) neutron absorber material of generation IV nuclear reactors: this is due to both the presence of ^{10}B isotopes and to the high structural stability under neutron irradiation. The increasing need of modifiable power plant power compatible with intermittent renewable energy production makes research on boron carbide based materials invaluable. Besides, boron carbide is the third hardest industrial material known after diamond and cubic boron nitride, and for this reason, it is used as a material for shielding applications. Its lightness makes it valuable for personal protections and it is used in bulletproof jackets for civilians and (sometimes tailored) armours for soldiers. However, despite the fact that it has the highest elastic limit among all ceramics under dynamical loading (Hugoniot of $\sim 15-17$ GPa), when impacted beyond its Hugoniot Elastic Limit (HEL), B_4C shows a gradual loss of strength.

The objective of this project is the development of new ceramic(s) guided by ab initio and thermochemistry calculations, with the purpose of achieving high mechanical properties in a domain of stresses where standard boron carbide fails. We target the exploration of new ideas for the modeling and innovative synthesis at high pressure (HP) and high temperature (HT) of ternary phases B_xCSi_y , in which silicon atoms are introduced to reinforce the tri-atomic C-B-C chains with the help of HP-HT. Indeed, so far, silicon has only been reported as a doping element at ambient pressure in the literature. Contrastingly, our preliminary calculations show that high pressure favors the thermodynamical stability of some of the compositions. HP-HT ex situ synthesis experiments will be performed at IMPMC and in situ by synchrotron XRD in the (P,T) conditions guided by calculations. Samples will be characterized by conventional techniques such as XRD, microscopy and Raman spectroscopy.

Techniques/methods in use: High pressure techniques, XRD, Raman

Applicant skills: Good levels in solid-state physics and/or chemistry, written/spoken English skills

Industrial partnership: Y/N (specify the company).

Internship supervisor(s) (name, email, phone, webmail):

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Possibility for a Doctoral thesis: Y/N (specify if already financed) Y (financed).