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Vickers hardness of boron subarsenide $B_{12}As_2$ has been predicted using three modern theoretical models and experimentally studied by microindentation. The polycrystalline material exhibits hardness of about 31 GPa, and hence $B_{12}As_2$ belongs to a family of (super)hard phases.

Keywords: boron subarsenide, hardness, bulk modulus.

Boron subarsenide $B_{12}As_2$ is icosahedral boron-rich compound possessing a fortunate combination of properties (wide energy band gap, high carrier mobility, extraordinary radiation sustainability, etc.) [1-3] that makes it a promising material for electronic devices operating under extreme conditions. In the present Letter we report the hardness and other mechanical properties of $B_{12}As_2$ from theoretical and experimental studies.

Vickers hardness (H_V) of boron subarsenide was predicted using three contemporary theoretical models of hardness, i.e. the thermodynamic [4], the Lyakhov-Oganov [5] and the Mazhnik-Oganov [6] models. The general thermodynamic model based on crystal structure and thermodynamic properties was used in the formulation developed for the particular case of boron-rich solids [7], while within Lyakhov-Oganov approach the strength of covalent bonding, degree of ionicity and topology of the crystal structure were considered. Mazhnik-Oganov model based on elastic constants was also used for evaluation of fracture toughness (K_{Ic}). The results are summarized in Table. It should be noted that bulk modulus of $B_{12}As_2$ estimated in framework of the thermodynamic model is in good agreement with the experimental value 150(4) GPa [8].

Stoichiometric $B_{12}As_2$ has been synthesized by the method described elsewhere [8]. Polycrystalline bulks for hardness measurements have been produced in a toroid-type apparatus by crystallization from melt at 5.2 GPa. According to X-ray diffraction study (TEXT 3000 Inel) the recovered bulks contain well-crystallized single-phase $B_{12}As_2$ with lattice parameters identical to the literature data [9].

The recovered samples were planar ground with diamond 800 grit and subsequently polished with 9-μm and 1-μm diamond suspensions. Final vibropolishing with 0.04-μm SiO_2 colloidal solution ensured the minimal sample surface damage.

According to scanning electron microscopy study (TESCAN MIRA3 FEG) all samples were homogeneous without residual porosity, and their grain size varied from 0.5 to 3 μm.

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Vickers hardness measurements have been performed using a Mitutoyo HM-220B Microhardness Testing Machine under loads from 1 to 20 N and 15 seconds dwell time; five indentations were made at each load. Hardness and indentation fracture toughness values were calculated following the standard definitions from the residual imprints upon indentation (for details see [12]).

The measured Vickers hardness of boron subarsenide decreases with the load, and at 6 N reaches the asymptotic value $H_V = 31(2)$ GPa that is in perfect agreement with the hardness calculated by the thermodynamic and Mazhnik-Oganov models (see Table). H_V value calculated using Lyakhov-Oganov model is slightly overestimated. Indentation fracture toughness is almost independent of the load, and the experimental value of $K_{Ic} = 1.1(3)$ MPa·m$^{0.5}$ is in agreement with the calculated one.

Thus, boron subarsenide $B_{12}As_2$ exhibits experimental Vickers hardness of 31(2) GPa which is higher than that of cubic silicon carbide SiC, a conventional superabrasive. All used theoretical models work properly, however, the thermodynamic model seems to be more reliable in the case of boron-rich solids.

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Table Mechanical properties of boron subarsenide: Vickers hardness (H_V), bulk modulus (B_0), shear modulus (G_v), Young's modulus (E), Poisson's ratio (ν) and fracture toughness (K_{Ic}).

H_V				B_0	G_v	E	ν	K_{Ic}
T [a]	LO [b]	MO [c]	exp.					
GPa							—	MPa·m^{½}
32	35	31	31(2)	158 [a]	168 [d]	367 [e]	0.092 [e]	1.3 [c]

[a] Thermodynamic model (particular case of boron-rich solids) [4,7].

[b] Lyakhov-Oganov model [5].

[c] Mazhnik-Oganov model [6].

[d] Calculated from elastic moduli C_{ij} [10] using Voigt's approach [11].

[e] Calculated from B_0 and G_v values using isotropic approximation.