Ab-initio INVESTIGATION OF La-Ba-B_6 ALLOYS

Ivashchenko V.I., Shevchenko V.I., Olifan E.I., Rud B.M.
Institute for Problems of Material Science, NAS of Ukraine (Dep. 7),
Krzhyzhanovsky str. 3, 0380 Kyiv-142, Ukraine,
e-mail: ivash@ipms.kiev.ua

Broad experience in the design of super-hard nanocomposites has been achieved during the last decade. It was shown that the high hardness of such nanocomposites was caused not only by the availability of grain boundaries, but also by the intrinsic strength of the materials of nanocomposites.

In this work we investigate the La-Ba-B_6 alloys as the perspective materials for superhard nanocomposite coatings using the first-principles pseudopotental "Quantum espresso" code. The cubic cells of $La_{8-n}Ba_nB_{48}$ alloys, n=1-8, with several possible configurations for each concentration were used in variable-cell structural relaxation and density of states (DOS) calculations.

In Fig. 1 we show the mixing energy of the alloys as a function of composition. The total DOSs of the alloys are presented in Fig. 2. The stress-strain curves for TiN, ZrN and La_8B_{48} (LaB_6) are shown in Fig. 3.

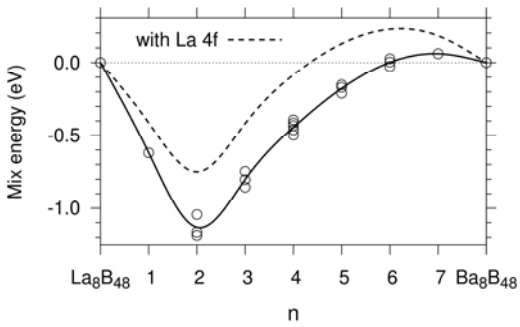

Fig. 1 Mixing energy ($E_{mix}(n)= E_T(La_{8-n}Ba_nB_{48}) – (8-n) \times E_T(La_8B_{48})-n\times E_T(Ba_8B_{48})$of the $La_{8-n}Ba_nB_{48}$ alloys as functions of the concentration n. The dashed line is the mixing energy calculated by taking into account the La 4f states

It follows from these findings that, in the La-Ba-B_6 system, the stable solid solutions $La_{8-n}Ba_nB_{48}$ can form in the range n>5. The value of the DOS at the Fermi level extracted from Fig. 2 (not shown here) drastic increases with substitution of Ba by La, which strongly destabilizes the alloys (cf. Fig. 1). The ideal shear strength of LaB_6 is comparable with that of TiN and ZrN, which indicates that LaB_6 and perhaps $La_{8-n}Ba_nB_{48}$ alloys, for n ≈ 2, can be used as the perspective materials with the high intrinsic strength for producing hard nanocomposite coatings.

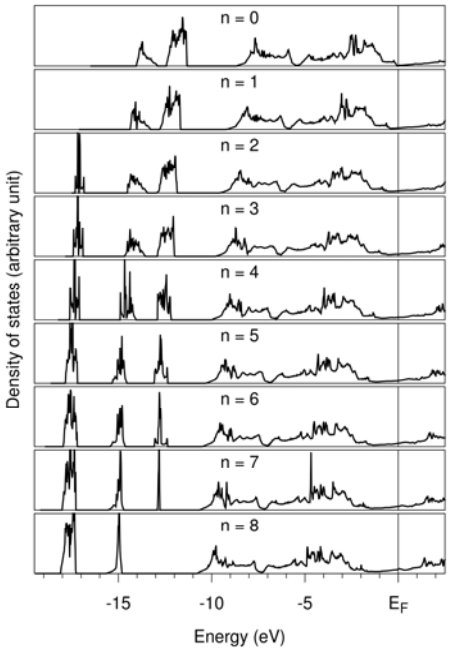

Fig. 2 Density of states (DOS) of the $La_{8-n}Ba_nB_{48}$ alloys as functions of the concentration n. The vertical line denotes the Fermi level (E_F). For each concentration n, only the DOS of the configuration with the smallest E_T is shown

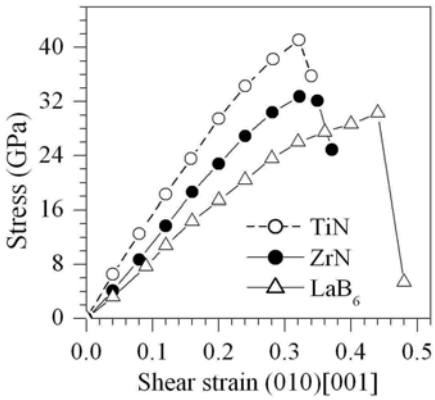

Fig. 3 Calculated stress-shear strain curves for TiN, ZrN and LaB_6