

## Phase stability of AlMgB14 based materials and Ge2Sb2Te5 with Si and N additions studied by theoretical and experimental means



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## PHASE STABILITY OF ALMGB14 BASED MATERIALS AND GE2SB2TE5 WITH SI AND N ADDITIONS STUDIED BY THEORETICAL AND EXPERIMENTAL MEANS

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Shaker Verlag Sep 2011, 2011. Taschenbuch. Book Condition: Neu. Neuware - The effect of valence electron concentration (VEC) and size of the X element in XMgB14 (space group Imma X=Al, C, Si, Ge, Mg, Sc, Ti, V, Zr, Hf, Nb, Ta) on stability and elastic properties was studied using ab initio calculations. Generally, icosahedral bonds, present in these compounds, are electron deficient. X elements and Mg are shown here to transfer electrons to the boron network. Hence, the stability of the compounds studied increases as more electrons are transferred. As the VEC of the X element increases, fewer electrons are transferred to the boron network, and therefore the phase stability decreases. The bulk moduli of all compounds are in the range from 205 to 220 GPa. This can be understood analyzing the cohesive energy thereof. As the bulk modulus increases, the cohesive energy decreases. Furthermore, AlYB14 (Imma) thin films were synthesized by magnetron sputtering. On the basis of x-ray diffraction, no phases other than crystalline AlYB14 could be identified. According to electron probe microanalysis, energy dispersive x-ray analysis, and elastic recoil detection analysis, the Al and Y occupancies vary in the range of 0.73-1.0 and 0.29-0.45, respectively. Density functional theory based calculations were carried out to investigate the effect of occupancy on the stability of Al<sub>x</sub>Y<sub>y</sub>B14 (x,y = 0.25, 0.5, 0.75, 1). The mean effective charge per icosahedron and the bulk moduli were also calculated. It is shown that the most stable configuration is Al<sub>0.5</sub>YB14, corresponding to a charge transfer of two electrons from the metal atoms to the boron icosahedra. Furthermore, it is found that the stability of a configuration is increased as the charge is homogeneously distributed within the icosahedra. The bulk moduli for all configurations investigated are in the range between 196 and 220 GPa, rather close...



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