ELASTIC CONSANTS FOR ALLOYS WITH MECHANICAL INSTABILITY: AB INITIO INVESTIGATION OF BCC Ti

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The influence of the amount content of V on the mechanical phases stability of body-centered cubic (bcc) based Ti-V alloys was studied. The elastic properties of the binary system of bcc Ti-V alloys were investigated using the non-empirical method of pseudopotentials and the method of exact MT orbitals in the entire concentration range of V. Disorder substitution was modeled using a special quasi-random structure (SQS) technique and in the coherent potential approximation (CPA). The concentration V dependence of the elastic constants of the single crystal $C_{\alpha\beta}$, obtained by calculating the total energy for the corresponding deformations, and also family of material characteristics E, B, G, Pc, k, v for the TiV system were introduced and discussed. In the case Ti-V alloys, a comparative analysis of efficiency of the PAW and EMTO methods to obtain data of the elastic properties of Ti-V alloys from the first-principle modeling over a wide range of the concentration V was presented. It was found that Ti-rich TiV alloys are mechanically unstable in the bcc phase, but at higher concentration V in the system the mechanical stability is increased. The efficiency of using different calculation methods in the study of the elastic properties of disordered alloys are discussed.