Αγγλική περίληψη

This diploma thesis is divided into two parts, the theoretical and the experimental. Initially, in the theoretical part, a brief introduction to the material TiB_2 is made. Then, the basic structural characteristics are presented briefly along with the physical and mechanical properties, which are exploited in numerous applications. Also some of the production methods of the bulk material and especially of its thin films, where the material shows overstoichiometry in boron, are listed. Additionally the DOS diagram, facilitates the explanation of the nature of the bonding between the constituents of TiB_2. Continuing in the theoretical part of this work, some details of the methodology are given. Specifically the basic ideas of Density Functional Theory (DFT) are described along with the methods that preceded it. A description of the pseudopotential and projector augmented waves (PAW) methods follows, along with the approaches that describe the interaction between the electrons. These are the theories underlying the study of structural and elastic properties of the material in this work. Then a brief introduction to grid computing and ab-initio software packages is made, with particular emphasis on the software package VASP (Vienna ab-initio simulation package). The above software package along with the implementation of the HellasGrid resources, were used in all calculations of this work. The experimental part of this work includes all the results of the calculations made. Initially, the structure of the material was simulated to study its structural characteristics. After using isotropic deformations of the primitive cell, the bulk modulus of the material was calculated, using the energy – volume data of the deformed structures. Then by applying anisotropic deformations, the five different elastic constants of TiB_2 were calculated, leading to the calculation of the material's elastic properties. In all the above calculations, results are compared to bibliography. At the end of the experimental section, overstoichiometric structures of TiB_2 ($2.000 < x < 2.104$) were simulated and their bulk moduli, elastic constants and properties were studied as above. A comparison of the calculated properties of overstoichiometric structures with those of stoichiometric TiB_2 follows. In conclusion some comments concerning the results of this thesis are given.