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A simple approach to the polytypism in boron nitride TOMONORI ITO, TORU AKIYAMA, KOHJI NAKAMURA, Department of Physics Engineering, Mie University — Boron nitride (BN) is well known as having a polytype including cubic (c-BN) with zinc blende structure (3C) and hexagonal BN (h-BN) phases similarly to C. From the experimental viewpoints, it is found that h-BN appears at ambient temperature and pressure whereas c-BN is preferable at high temperature and high pressure. In order to clarify its polytypism, there have been some ab initio calculations mainly focusing on four-fold coordinated structures such as 3C-, 6H-, 4H-, and 2H-BN. Although the ab initio calculations predict the polytypes for bulk BN, the physical interpretation of the polytypism is still unclear because of the complexity of identifying individual contribution in the ab initio calculations. In order to make up this deficiency, we investigate the polytypism for BN in bulk form using a simple approach on the basis of empirical interatomic potentials. The calculated respective energy differences between 6H and 3C, between 4H and 3C, and between 2H and 3C are 5.0 meV, 7.5 meV, and 17.1 meV when the ionicity fi=0.143 for BN is employed. These results are consistent with previously reported ab initio calculations. Furthermore, we also discuss the relative stability between h-BN and c-BN using this simple approach.

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