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Structural properties and phase stability of Ti alloys containing V and Cr by first-principles calculation LINGGANG ZHU, BENGT TEGNER, GRAEME ACKLAND, SUPA, School of Physics and Astronomy, The University of Edinburgh, QING-MIAO HU, RUI YANG, Shenyang National Laboratory for Materials Sciences, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China — We apply the first-principles plane-wave pseudopotential method and virtual crystal approximation (VCA), to investigate structural properties and phase stability of ternary titanium alloy Ti-V-Cr. The lattice parameters of the alloy vary almost linearly with the number of d electrons in spite of the different ratio of V to Cr, which agrees with the available experimental results. At 0K, we find that an extra 0.4 electrons per atom can stabilise the beta Ti-V-Cr. Debye approximation is used to consider the temperature effect, and it is found that at 973K, with an extra 0.1 d electron per atom, the beta Ti-V-Cr can be stabilised, compared with 0.15-0.20 d electron required experimentally at 973K. It is shown that V and Cr move the Fermi energy to lower values of the density of the states of the beta phase, which accounts for the stabilisation effect.

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