Effects of Misfit Dislocations on the Band Alignment of Zincblende Semiconductors

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The band offset largely determines electrical transport across heterointerfaces in electronic and optoelectronic devices. Its accurate determination has therefore been one of the long-standing problems in computational materials science. The band offset by nature depends on the atomistic and electronic structure of the heterointerface. Assuming such dependences to be weak at interfaces composed of structurally and chemically similar materials, a band alignment diagram, where relevant materials are aligned using a common reference level, carries information of the band offsets to a large extent.

Quantities such as branch points from bulk calculations and ionization potentials from surface calculations, as well as band offsets explicitly obtained from interface calculations, have been used for the alignment[1-7]. However, the effects of misfit dislocations at semicoherent interfaces have typically been neglected.

Actual semicoherent interfaces have two-dimensional dislocation networks with an inter-dislocation distance determined by the misfits and the Burgers vectors, but it is not feasible to explicitly treat such interfaces in supercells for first-principles calculations. Therefore, an interface with a one-dimensional array of misfit dislocations can be considered instead. In such a model, the number of atoms per supercell is significantly reduced.

Figure 1(a) shows a 462-atom supercell model of perfect edge dislocations at the CdS/ZnS (110) interface with Burgers vector $\mathbf{b} = \frac{a}{2}[1\bar{1}0]$ and line vector $\boldsymbol{\xi} = [001]$. There are five-fold coordinated Cd and three-fold coordinated Zn atoms at the dislocation as shown in the enlarged figure [Fig. 1(b)], and no dislocation-induced electronic states are observed in the band gap [Fig. 1(c)] [1]. The CdS/CIS band offset, according to the simplified natural band offset definition [2], is -0.01 eV without the dislocation and -0.05 eV with the dislocation, indicating that the band offset is not significantly influenced from this type of misfit dislocations [1].

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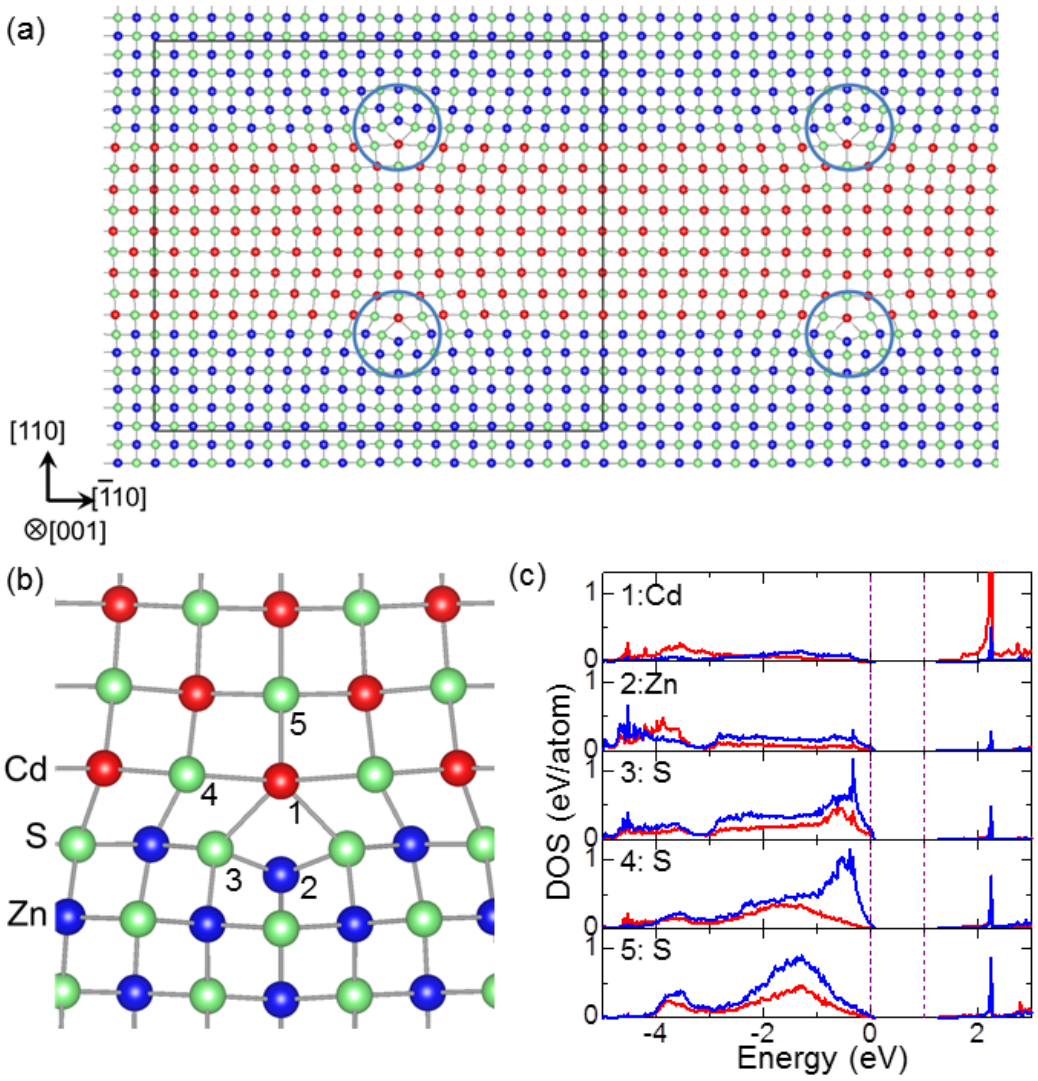

FIG. 1. (a) Structure of CdS/ZnS (110) interface supercells containing perfect edge dislocations with a Burgers vector of $\frac{a}{2}[1\bar{1}0]$ and a line vector of $[001]$. The black frame represents the supercell and the dislocations are enclosed by circles. (b) Core structure of a dislocation. (c) Site-projected electronic DOS in the vicinity of dislocation cores. The numbers correspond to those indicated in (b).The thick red and thin blue curves show *s* and *p* orbital components, respectively. The dashed lines show the higher VBM and lower CBM of the two phases estimated from bulklike regions far from the interface; the former is taken as the zero of the energy [1].