Stain energy calculation in ZnTeO semiconductor alloys by VFF method

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Valence force field method (VFF)[1,2] is an algorithm used to calculate the strain energy. The basic idea of VFF method is to approximate the potential energy of a crystal by considering the interactions between atoms.

The substitution of Te by O in ZnTe results in a smaller bond length for oxygen compared to tellurium. This mismatch leads to high lattice misfit and significant internal strain in the material, which can negatively affect the properties of the device so, we calculate the strain energy of ZnTeO with VFF.

The size of crystal 100×100×100 in[110],[$1\bar{1}0$]and[001]directions.The oxygen content is randomly distributed in the crystal.

Newton's method is an iterative technique used to change the position of every atom for minimization of the total strain energy in the crystal.

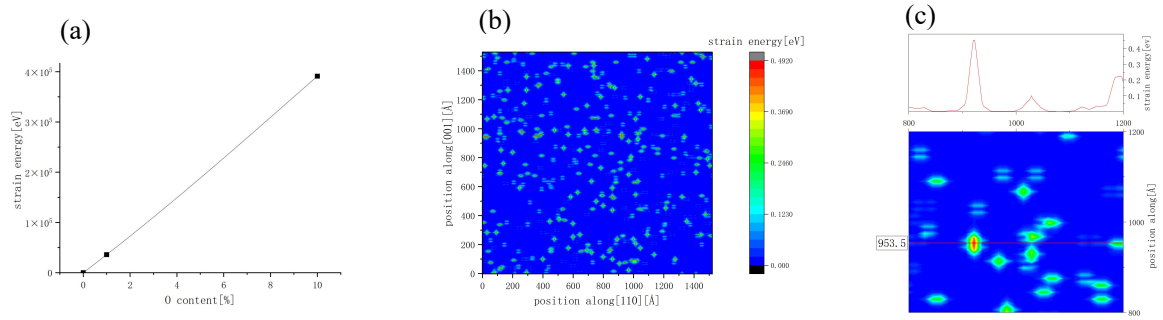

Fig. 1.(a)total strain energies in crystals with different O contents. (b)Strain energy distribution in a ($1\bar{1}0$) plane. (c) The profile plot of the strain energy.

The calculated results depicted in Fig. 1 reveal that the introduction of oxygen atoms into the lattice causes a highly concentrated distribution of strain energy in the oxygen-substituted region, significantly disturbing the local lattice structure, and that the total strain energy increases rapidly with the oxygen content, suggesting that greater oxygen doping levels lead to more severe lattice mismatch and internal strain issues.

1P. N. Keating, Phys. Rev. 145,637 1966.

2R. M. Martin, Phys. Rev. B 1, 4005 1970.