

Abstract Submitted
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Modeling Rotation of H in Cu-H Defect Complex in ZnO AN-DREW MAGYAR, Ohio Northern University — The rotational motion of the bond-centered H or D atom in an isolated Cu-H defect complex in the ZnO crystal lattice is modeled under uniaxial stress. The uniaxial stress is applied along the c-axis of the crystal and causes an absorption line at 3229 cm^{-1} to appear and then increase in intensity under increased stress. The behavior of this line, and the characteristic line of the defect at 3192 cm^{-1} , are studied. Our model assumes that stressing the crystal breaks the rotational symmetry of the H atom, causing the rotational states to mix together. Under these assumptions, the model is able to match experimental data collected by Lavrov and Weber. Methods for selecting parameters of the model are discussed, along with the behavior of the probability function of the H or D atom.

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