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Doping effect of alkali metal elements on the structural stability and transport properties of ZnO at high pressures

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ABSTRACT

In this paper, we report the tuning effects on the structural stability and transport properties of ZnO under high pressure at room temperature after doping it with a series of alkali metal elements (Li, Na, and K). Generally, substitution at the Zn site (with the large ionic radii of the 1st group elements) leads to *p*-type conductivity with an increase in the Zn-O bond distance. Whereas, the external high pressure compresses the crystallite size, leading to increased lattice strain and band gap reduction in this semiconductor material. As a result of lattice strain hindrance upon compression, the larger ions rather than the smaller ions try to counteract the high pressure due to ionic force repulsion within the lattice. By combining synchrotron x-ray diffraction, Raman spectroscopy and *insitu* resistant measurements under pressure on Li-, Na-, and K-doped ZnO nanomaterials, we demonstrated that the critical phase transition pressure of ZnO from wurtzite to rock salt changes from 9 GPa to 13 GPa, and a resistance change anomaly occurs around these transition pressures. This study of the structural, vibrational stability and transport properties of a series of alkali metal element-doped ZnO under pressure provides an efficient way to modify these types of semiconductor materials for technological applications.

Keywords:

semiconductor; phase transition; high-pressure; synchrotron x-ray diffraction