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Unusual uniaxial stress results on the stretch mode of OH related defects in ZnO KEVIN MARTIN, University of Pittsburgh at Johnstown, Johnstown PA, W. BEALL FOWLER, Lehigh University, Bethlehem PA — Some uniaxial stress studies of the frequency dependence of O-H-related defects in ZnO have produced surprising results[1,2]. For example, the Li:OH defect in ZnO (H-I*) is oriented along the c-axis, yet the OH stretch mode decreases in frequency when stress is applied along the c direction and increases when stress is perpendicular to the c-direction. Another example is the Cu:OH defect, in which the OH is aligned along one of the three non-c tetrahedral directions. Stress along the c-direction produces a strongly non-linear increase in frequency. These examples and others indicate something unusual is happening in these systems. One possibility is that the piezoelectric effect in ZnO is responsible for the "backward" behavior of the frequency shift of these defects. The piezoelectric effect in ZnO is caused by the lack of cancellation between the "clamped-ion" term (i.e., electronic contribution) and the term related to the change in the u parameter ("internal strain"), with the latter dominating[3]. When c stress is applied, the value of u increases, thus the two interpenetrating hexagonal lattices (one for Zn, the other for O) increase their overlap. We will attempt to explain the experimental results within this framework.
[1]Lavrov and Weber, Phys. Rev. B, **73**, 035208 (2006), and [2] Phys.Stat. Sol. (b) **243**, 2657 (2006) [3]Corso, et al Phys. Rev B. **50**, 10715 (1994)

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