Vibrational properties of the As deposited InP(110) surface

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We report on the vibrational properties of arsenic deposited InP(110) surface, based on investigations carried out using an adiabatic bond charge model. As arsenic deposition at room temperature is likely to result into an As–P exchange [1], we have studied the lattice dynamics of the As/InP(110)-(1×1) system using two structural models: epitaxially continued layer structure and an exchange-reacted structure. The structural and electronic information necessary for these calculations is obtained using the *ab initio* pseudopotential method. For both structural models we find that deposition of As on InP(110) results in several characteristic new phonon modes in the bulk acoustical-optical gap range. However, it is found that for the exchange-reacted geometry there is still a clear gap of approximately 10 meV in the bulk acoustical-optical gap region. Our results agree well with the Raman scattering measurement and a previous first-principles calculation for the zone-centre surface phonon modes [1]. To the best of our knowledge, this work is the first surface dynamics calculation for the epitaxially continued layer structure of As:InP(110). A collective analysis of the structural, electronic and vibrational results for the two models will be made to point out signatures of well ordered versus poorly ordered As overlayer on InP(110).

[1] U. Grossner, W. G. Schmidt and F. Bechstedt, Phys. Rev. B **56**, 6719 (1997).