Abstract Submitted
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Theoretical study of adsortion of Sb on GaAs(110) surface[1] NORBERTO ARZATE, RAUL VAZQUEZ, BERNARDO MENDOZA, Centro de Investigaciones en Optica, A. C. — We present a model for studying the adsorption of Sb atoms on a clean GaAs(110) surface and analyse the consequences of the adsorption on the reflectance anisotropy spectroscopy (RAS). A 1×3 unit cell is taken as a basis of the Sb-covered GaAs(110) structure. The relaxed coordinates of each configuration have been obtained thanks the use of the ABINIT code [1,2], that is based on pseudopotentials and planewaves. We allow the Sb-covered surface to be disordered by letting every surface atom move freely around its equilibrium position. In order to obtain a representative RAS spectrum of the surface we generate an ensemble with $\mathcal{N}$ different structural realizations of the surface and the ensemble RAS average is performed.
[1] X. Gonze, et al., Computational Materials Science **25**, 478 (2002).
[2] X. Gonze, et al., Zeit. Kristallogr. **220**, 558 (2005).
[3] Bernardo S. Mendoza, N. Arzate and R.A. Vázquez-Nava, phys. stat. soli. (c) **2**, 4031 (2005).

[1]SEP-2004-C01-48142 and SEP-2003-C02-42576.

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