Vibrational Properties of Homopolar and Heteropolar Surfaces and Interfaces of the CdTe/HgTe System

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We present results of calculations for the density of vibrational modes for (001) and (111) homopolar, as well as for (011) heteropolar free surfaces of CdTe and HgTe. A rigid-ion model with a dynamical matrix parametrization including force constants up to second neighbours is used. The interface atomic planes show themselves as plionon gapless layers. Tlie contribution of in-plane and out-of-plane vibrations is analysed for both the surface and iiiterface cases.

The study of the physics of surfaces, interfaces, and superlattices of 11-VI semiconductors is drawing new and increasing interest nowadays. At tlie origin of a. deep understanding of the experimental results on these systems is an accurate description of tlieir electroiiic structures and their phonon spectra. Vibrational properties of CdTe/HgTe heterostructures start just to be considered[1,2], in spite of the paramount importance of phonons to obtain a reliable tlieoretical description of the main optical and transport features of this system, where the overlapping in energy of electronic intra- and inter-band transitions with phonons must be taken into account. Bulk phonons of some II-VI semiconductors have been only recently studied, from tlie theoretical side, by ab initio calculations by Dal Corso et al.[3]. The ab initio calculations are the most appropriate answer to this problem but it is far from realistic now to apply it to heterostructures. Therefore, yet another method of calculation, which allows an easy and quick test of models, hypothesis, and geoinetrical situations, has proven desirable. It is the purpose of this paper to illustrate the use of a very simple one that takes full advantage of the existing ingredients for tlie calculation of the phonon spectra for surfaces and interfaces of semiconductors. Using the Green's Function theory, we explore tlie possibilities of various surface and inter-

face induced vibrational modes. The Green's function technique we employ, adapted to layer geometries, has been used previously by the authors in the study of the electronic properties of the surface and quantum wells for tliis sarne system[4,5].

We will concern ourselves with a rigid-ion model because of its simplicity. Here we consider a 8 parameter phenomenological model for the description of the lattice dynamics of CdTe and HgTe[6] iwhich has proven useful in the study of the HgCdTe alloy. First- and second-nearest- neighbour force constants are included. For the illustrative calculations in this paper, the interfacial force constants are taken to be equal to the geometric mean of the force constants for the materials which form the interface. This choice is motivated by simplicity. We shall consider ideal (no reconstruction, no relaxation, no clisorder) free surfaces, perpendicular to the (001), (011) and (111) directions. For these same directions ideal lattice-matched interfaces are studied. The choice and labeling of in-plane and out-of-plane axis are despicted in Fig. 1.

In spite of the importance of the long-range Coulomb forces we ignore these forces for describing tlie lattice dynamics of this system. The effects of the long-range Coulomb forces are significant only in the long- wavelength limit; the direct effect on the global

features of the densities of phonon states can be considered to be fairly small[7].
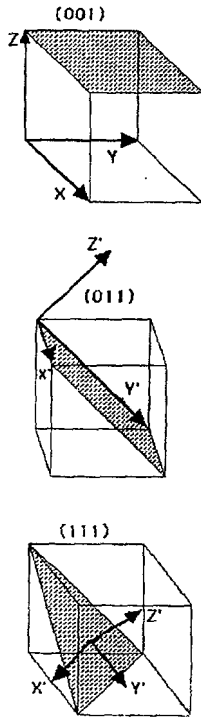

Figure 1: She choice and labeling of in-plane and out-of-plane axis for each main direction.
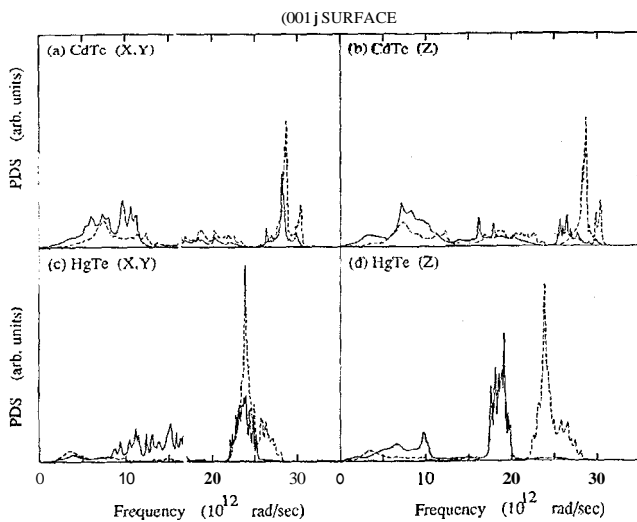

Figure 2: Phonon density-of-states (PDS) of anion terminated (001) surface: (a) CdTe, in-plane vibrations; (b) CdTe, out-of-plane vibrations; (c) HgTe, in-plane vibrations; (d) HgTe, out-of-plane vibrations. Solid line: surface layer; dashed line: bulk layer.
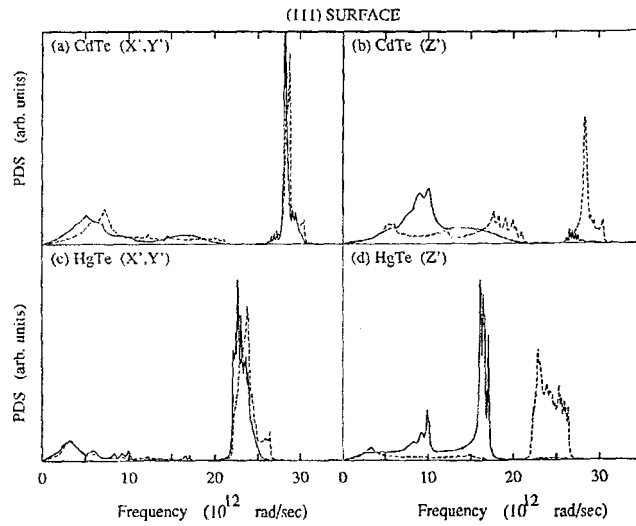

Figure 3: As in Fig. 2, but for the (111) surface.

We discuss first homopolar surfaces. The phonon density-of-states (PDS) is shown in Fig. 2 for (001) anion terminated surfaces. In-plane vibrations are practically unaffected by the free surface in CdTe, Fig.2 (a), while they show large modifications in the case of HgTe, Fig.2 (c). For the other polarization, out-of-plane vibrations, a shift of spectral weight from the optical region to the acoustical one is observed in CdTe, Fig.2 (b). In contrast, the HgTe-surface shows a strong shift of spectral weight from the optical branch to the phonon gap Fig.2 (d), filling the large gap of the perfect crystal. This fact maltes of the HgTe-surface a phonon gapless layer. For the other homopolar surface (111) it is to be noted essentially the same kind of behaviour for the CdTe semiconductor as it is shown in Fig. 3(a,b). The HgTe (111) free surface shows a large shifting of spectral weight in the case of out-of-plane vibrations, Fig. 3(d). A small gap is now open between acoustical and optical phonon branches. These surfaces show a beliaviour so different due to the large difference of masses between light Cd atoms and heavy Hg atoms. Therefore, for homopolar free surfaces of HgTe the perturbation is so strong that an important modification of the phonon spectra takes place.
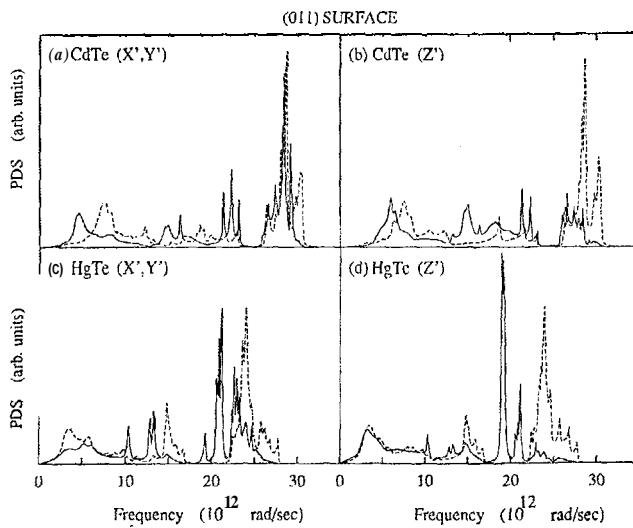
(011) SURFACE

Figure 4: As in Fig. 2, but for tlie (011) surface.
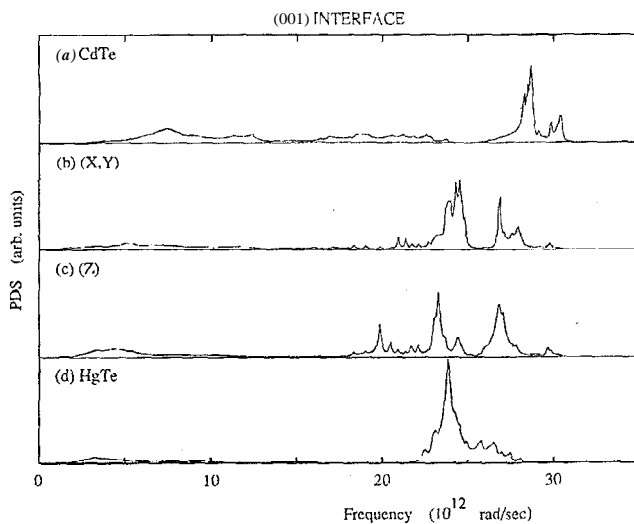
(001) INTERFACE

Figure 5: Phoiion density-of-states (PDS) of anion layers for tlie (001) CdTe/HgTe interface. (a) CdTe bulk layer; (b) in-plane vibration at interface layer; (c) oiit-of-plane vibration at interface layer; (d) HgTe bulk layer.
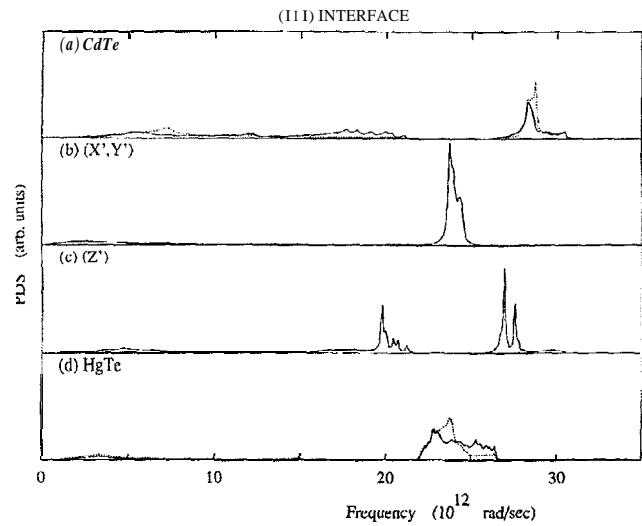
(111) INTERFACE

Figure 6: Phonon density-of-states (PDS) of anion layers for the (111) CdTe/HgTe interface. (a) CdTe bulk layer; (b) in-plane vibration at interface layer; (c) out-of-plane vibration at interface layer; (d) HgTe bulk layer. Solid lines denote oiit-of-plane polarization and dotted lines denote in-plane polarization for bulk Iayers.

The PDS for tlie heteropolar surface (011) is despicted in Fig. 4, for each material. The CdTe surface, Fig. 4(a,b), shows in this case tlie presence of both in-plane and out-of-plane polarized resonances at tlie top of the acoustical brancli, a feature not present in the hoinopolar surfaces. As before, the out-of-plane vibrations present a strong weight shifting from the optical to the acoustical region. In the same way, tke HgTe surface, Fig. 4(c,d), has higli localized modes at the phonon gap of the bulk material.

Another kind of perturbation is proposed by the interface. Fig. 5 shows the PDS of an ideal (001) CdTe/HgTe interface, Fig. 5(b,c) as compared with tlie layer PDS of the bulk materials, Fig. 5(a,d). It is important to point out that while in bulk zincblende crystals, tlie x, y, and z vibrations are equivalent due to the cuhic symmetry, at the interface layer in-plane and out-of-plane vibrations offer a very different spectrum. Bulk in-plane vibration features of CdTe and HgTe are still present in the interface anion layer but slightly shifted. In contrast, the out-of-plane vibration spectrum at the interface layer shows some features not present in neither of the bulk layers. A new peak develops at a frequency around 20×10^{12} rad/sec corresponding to a low density region of acoustical modes in bulk CdTe and the phonon gap of bulk HgTe. In addition, the interface layer shows itself as a phonon gapless layer. This behaviour is similar, but less pronounced, to that found at the HgTe (001) free surface. The other homopolar interface, (111), presents a PDS as shown in Fig. 6. In this case it is not valid that x', y' and z' vibrations are equivalent in bulk layers. This is explicitly marked in Fig. 6(a,d) where the in-plane and out-of-plane bulk densities of vibrational modes are separately

drawn. The interface PDS shows again an out-of-plane polarized new feature at a frequency smaller than any of the optical ones of each semiconductor.
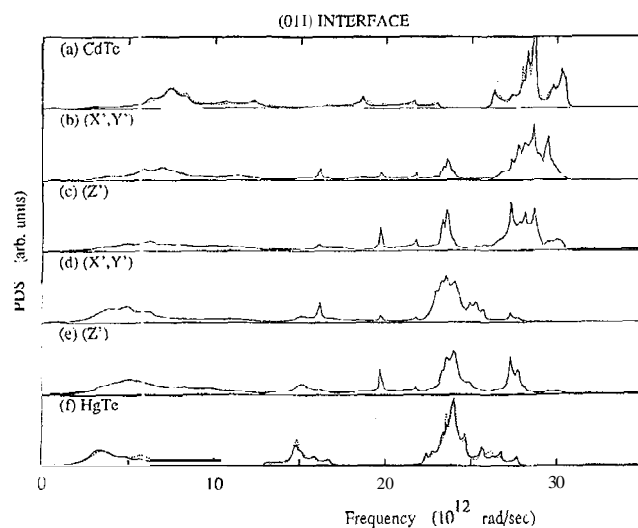

Figure 7: Phonon clensity-of-stales(PDS) of heteropolar layers for the (011) CdTe/HgTe interface. (a) CdTe biilk layer; (b) in-plane vibration at the CdTe interface layer; (c) out-of-plane vibration at the CdTe iiiterface layer; (d) in-plane vibration at the HgTe interface layer; (e) oiit-of-plane vibration at the HgTe interface layer; (€) HgTe biilk layer. Solid lines denote out-of-plane polarization and dotted lines denote in-plane polarization for biilk layers.

The PDS of the heteropolar interface (011) is illustrated in Fig.7. Ill this case there is not a. common atomic plane between the two inaterials. The interface is then more abrupt than in the homopolar cases. This is evident from Fig.7 (b,c) where in-plane and out-of-plane vibrations of the intcrface layer on the CdTe side, are very diflèrent of the similar one on the HgTe side, Fig.7 (d,e). The two interface layers have not any more phonon gaps, as compared witb tlie bulk layers density of states despicted in Fig.7 (a,f).

In summary, we have studied the main phonon properties of homopolar (001), (111), and heteropolar (011) free surfaces and lattice-matched interfaces of CdTe and HgTe semiconductors. We have shown how using a simple dynamical matrix parametrization in the framework of the rigid-ion model a great deal of information can he obtained about the vibrational properties of these important materials. 111-plane and out-of- plane polarizations have been systematically analysed for each orientation of tlie surfaces and interfaces. Of tlie two materials studied, HgTe presents the more dramatic variations in its vibrational features as a surface or interface is developed.

Acknowledgements

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