# Atomistic Modeling of the Structural and Thermal Conductivity of the InSb

José Pedro Rino<sup>1</sup>, Giovano de Oliveira Cardozo<sup>1</sup> and Adalberto Picinin<sup>1</sup>

**Abstract:** A new parametrization for the previous empirical interatomic potential for indium antimonite is presented. This alternative parametrization is designed to correct the energetic sequence of structures. The effective empirical interatomic potential proposed consists of two and three body interactions which has the same functional form of the interatomic potential proposed by Vashishta et. al. to study other semiconductors (Branicio *et al.*, 2003; Ebbsjo *et al.*, 2000; Shimojo *et al.*, 2000; Vashishta *et al.*, 2008). Molecular dynamics simulations (MD) are performed to study high pressure phases of InSb up to 70 GPa and its thermal conductivity as a function of temperature. The rock-salt to cesium chloride, expected to occur at high pressures, is observed with the proposed interatomic potential.

## 1 Introduction

The interest in developing empirical interatomic potential for materials is still very important. These empirical potentials express the total energy of the system of atoms as a function of its atomic positions. The most important feature of a good empirical potential is not only it accuracy but also its transferability (Brenner, 2000). The importance of a potential function relies on simplification of the quantum mechanics and ab initio complexity. These simplifications are very important once it can provide analytical solutions of materials properties (Chiang *et al.*, 2008). In particular for semiconductors, elemental or not, several empirical potential has been proposed (Branicio *et al.*, 2003; Brenner, 2000; Chakrabarty and Cagin, 2008; Chatterjee *et al.*, 2000; Erkoç, 1997; Rino *et al.*, 2002; Stillinger & Weber, 1985; Tersoff, 1988a; Tersoff, 1988b; Tersoff, 1988c).

In particular for indium antimonite Costa et al (Costa *et al.*, 2002; Costa *et al.*, 2003) had proposed an empirical interatomic potential, based on the Vashishta-Rahman potential, (Vashishta and Rahman, 1978) in which the structural phase transition from zinc blend to rock salt induced by pressure was presented. Unfortunately the parametrization of these interatomic potentials, besides describing

<sup>&</sup>lt;sup>1</sup> Departamento de Física, Universidade Federal de São Carlos, 13565-905 São Carlos, SP – Brazil

correctly the first structural transformation and some dynamical properties, do not describe correctly the stability of the structures for this material as well as the other structural transformation at high pressures.

In this paper a new parametrization for InSb is presented but keeping the same functional form for the interatomic potential used before. Phase transformation induced by hydrostatic pressure and thermal conductivity as a function of temperature are then analyzed.

### 2 The interatomic potential

The energy is modeled as a sum of two and three body interactions. The pair potential includes Coulomb, steric repulsion, charge-dipole and dipole-dipole interactions. The three body interactions consider bond bend and bond stretching. The total energy interatomic potential reads:

$$\Phi = \sum_{i < j} \varphi_{ij}^{(2)}(r_{ij}) + \sum_{i,j < k} \varphi_{jik}^{(3)}(r_{ij}, r_{ik})$$
(1)

where

$$\varphi_{ij}^{(2)}(r) = \frac{H_{ij}}{r^{\eta_{ij}}} + \frac{Z_i Z_j}{r} e^{-r/\lambda} - \frac{D_{ij}}{2r^4} e^{-r/\xi} - \frac{W_{ij}}{r^6}.$$
(2)

and

$$\varphi_{jik}^{(3)}(r_{ij}, r_{ik}) = R^{(3)}(r_{ij}, r_{ik}) \cdot P^{(3)}(\theta_{jik}),$$
(3)

where

$$R^{(3)}(r_{ij}, r_{ik}) = B_{jik} \exp(\frac{\gamma}{r_{ij} - r_0} + \frac{\gamma}{r_{ik} - r_0}) \Theta(r_0 - r_{ij})\Theta(r_0 - r_{ik})$$
(4)

$$P^{(3)}(\theta_{jik}) = \frac{\left(\cos\theta_{jik} - \cos\bar{\theta}_{jik}\right)^2}{1 + C_{jik}\left(\cos\theta_{jik} - \cos\bar{\theta}_{jik}\right)^2}.$$
(5)

The two body term of the potential is truncated at  $r_{cut}$  and shifted for  $r < r_{cut}$  in order to have the potential and its first derivative continuous at the cutoff distance (Allen and Tildesley, 1987; Nakano *et al.*, 1994). The shifted pair potential is given by

$$\varphi_{ij}^{(2shifted)}(r) = \begin{cases} \varphi_{ij}^{(2)}(r) - \varphi_{ij}^{(2)}(r_{cut}) - (r - r_{cut}) \left( d\varphi_{ij}^{(2)}(r) / dr \right)_{r=r_{cut}} & r \le r_{cut} \\ 0 & r > r_{cut} \end{cases}$$
(6)

Here  $r \equiv r_{ij} = |\vec{r}_i - \vec{r}_j|$  is the distance between  $i^{th}$  atom at position  $\vec{r}_i$  and  $j^{th}$  atom at position  $\vec{r}_j$ , and  $\lambda$  and  $\xi$  are the screening lengths for Coulomb and chargedipole terms, respectively,  $\theta_{jik}$  the angle formed by  $\vec{r}_{ij}$  and  $\vec{r}_{ik}$ , and  $C_{jik}$  and  $\bar{\theta}_{jik}$  are constants.  $\Theta(r_0 - r_{ij})$  is the step function.

Table I summarizes the values for the strength of the steric repulsion,  $H_{ij}$ , the effective charge (in units of the electronic charge |e|), $Z_i$ , the strength of the chargedipole attraction,  $D_{ij}$ , the van der Waals interaction strength,  $W_{ij}$ , the exponents of the steric repulsion term,  $\eta_{ij}$ , and the strength of the three body interaction  $B_{jik}$ .

			In	Sb				
	$Z_i(e)$		0.8167 (0.9318)	-0.8167 (-0.9318)				
Two-body	$\lambda = 7.0 (5.0) \text{ Å}$		$\xi$ =3.75 (3.75) Å	$r_{cut} = 10.9 (7.5) \text{ Å}$		$e = 1.602 \times 10^{-19} \text{ C}$		
			In-In	In-Sb		Sb-Sb		
	$\eta_{ij}$		7 (7)	9 (9)		7 (7)		
	$H_{ij}$ (erg.Å <sup><math>\eta</math></sup> )		9.6284 $\times 10^{-10}$	$2.2422 \times 10^{-8}$		$7.3083 \times 10^{-9}$		
			$(5.5933 \times 10^{-10})$	$(2.4105 \times 10^{-8})$		$(1.2022 \times 10^{-8})$		
	$D_{ij}$ (erg.Å <sup>4</sup> )		0	$1.54061 \times 10^{-11}$		$3.08122 \times 10^{-11}$		
			(0)	$(6.0164 \times 10^{-11})$		$(12.0327 \times 10^{-11})$		
	$W_{ij}(\text{erg}.\text{\AA}^6)$		0 (0)	$14.041 \times 10^{-10}$		0 (0)		
				$(14.539 \times 10^{-10})$				
Three-body			$B_{jik}(erg)$	$\bar{\theta}_{jik}(^{o})$	$C_{jik}$ (	Å)	γÅ)	$r_0$ (Å)
		In-Sb-In	$6.840 \times 10^{-12}$	109.4712	8.7		1	3.8
			$(7.83 \times 10^{-12})$	(109.4712)	(40)		(1)	(3.8)
		Sb-In-Sb	$6.840 \times 10^{-12}$	109.4712	8.7		1	3.8
			$(7.83 \times 10^{-12})$	(109.4712)	(40	)	(1)	(3.8)

Table 1: Parameters for two- and three-body parts of the interaction potential used in the MD simulation. The old set of parameters is also displayed in parenthesis.

Table 2: Selected experimental quantities used to parameterize the interatomic potential.

		MD	Experiments <sup>(*)</sup>
a (Å)	6.473	6.473 (at 173K)	
Cohesive energy (eV	2.800	2.795	
Bulk modulus (GPa)	45.68	45.63	
	C <sub>11</sub>	65.8	65.7
Elastic Constants (GPa)	C <sub>12</sub>	35.7	35.6
	C <sub>44</sub>	43.4	25.2

(\*) See Refs. (Harrison, 1980; Madelung et al., 1982).

All simulations reported here were done in NPT ensemble with systems containing 1000, 10648, and 110512 particles. The equations of motion were integrated using velocity Verlet algorithm with a time step of 1.5fs.

As before, the parametrization was determined by fitting cohesive energy, bulk modulus, the lattice constant, and the elastic constant. Table II display the experimental and the values obtained by the simulation with the new parametrization.

Figure 1 shows the energy per particle *versus* volume per particle for Zinc Blend (ZB), Wurtzite (W), Rock Salt (RS), and Cesium Chloride (CsCL) structures. Using previous parametrization wurtzite phase was more stable than ZB. Here ZB is more stable than wurtzite by 3.4 meV/N.



Figure 1: Total energy per particle as a function of the volume per particle for wurtzite, zinc blende, rock salt and cesium chloride structures ( $Å^3$ ).

Further validation of the model was obtained by calculating the vibrational density of states as shown in Fig. 2. The deformable-bond approximation (DBA), (Bilz & Kress, 1979; Kunc *et al.*, 1975) which is based on the experimental phonon dispersion relation reported by Price et al., (Price *et al.*, 1971) are in good agreement with the calculated density of states. Once the results from the simulation reproduce very well these quantities, all parameters in the interatomic potential are kept constant to simulate other properties.

#### 3 Phases Transformation under hydrostatic pressure

Starting with a zinc blend phase at fixed temperature, the external pressure was increased in steps of few MPa every 2000 time steps, up to 70 GPa. Figure 3 below shows the reduced volume  $V/V_0$  as a function of the external pressure ( $V_0$  is the



Figure 2: Vibrational density of states calculated at 300K along with deformable-bond approximation results (Bilz & Kress, 1979; Kunc *et al.*, 1975).



Figure 3: Volume fraction as a function of pressure.  $V_0$  is the volume at zero pressure. Experimental results are from Ref. (Vanderborgh *et al.*, 1989).

volume at zero pressure). The ZB structure is dynamically stable up to 3.0GPa, and the agreement with experimental result of Vanderborgh et al (Vanderborgh *et al.*, 1989) is very good. The inset display the equation of state for the ZB phase.

The sudden drop in volume around 3GPa indicates that a first order phase transition took place. Pair distribution function, coordination number and bond angle distribution just before and after the transformation indicates that the new phase has features of a rock salt structure – see Figs. 4. A further increase in pressure causes new drop in volume at 49GPa, and a new first order transformation occurs. Structural characterization using two and three body correlations (Figs.5) indicates that this new phase has features of a cesium chloride structure. The CsCl phase is stable up to 70GPa (the maximum simulated pressure) and the backward transformation occurs with a large hysteresis, back transforming to RS at 20 GPa. Further reduction in pressure shows that the RS phase is stable up to 0GPa. It has been conjectured that the CsCl should be the natural high pressure phase, but as far as we know it has never been confirmed experimentally. (Mujica *et al.*, 2003).

Figure 6 depict the In-Sb bond distance defined as the peak position of the partial In-Sb pair distribution function as a function of the applied pressure. Up to 3GPa the system responds elastically under compression followed by a sudden increase in bond length at the transformation to the new phase. Further increase in pressure the elastic compression is again observed when around 49 GPa another phase transformation occurs as is shown by the new sudden increase in bond length. Up to 70GPa the system responds elastically. The backward transformation CsCl to RS structure shows a large hysteresis, but the RS phase remains stable up to zero pressure.



Figure 4: (a) In-Sb pair distribution function and coordination number, (b) In-Sb-In bond angle distribution for pressures just below and after the first structural transformation.



Figure 6: In-Sb bond length as a function of pressure. Large changes in bond length explicitly display the ZB to RS and from RS to CsCl transitions.



Figure 5: (a) In-Sb pair correlation function and coordination number, (b) In-Sb-In bond angles for pressures just above and below the second structural phase transition.



Figure 7: Heat current auto correlation function, calculated at T = 300K, as a function of time. Averages were taken over 1500 samples.

#### 4 Thermal Conductivity

Due to the good description obtained with the proposed interatomic potential in describing the sequence of structures, the ZB structural and dynamical properties as well as its pressure induced transformation, motivated us to use this empirical potential to study thermal conductivity in this system.

Thermal conductivity coefficients can be obtained using a fast Monte Carlo simulator for phonon transport, (Huang *et al.*, 2009) with equilibrium molecular dynamics (Cahill *et al.*, 2003) simulations or non-equilibrium molecular dynamics methods (Schelling *et al.*, 2002) among others. The equilibrium MD is based on Green-Kubo (Kubo, 1957) relations, and the non-equilibrium MD is the direct method where the Fourier law is used (Baranyai, 1996; Baranyai, 2000; Baranyai, 2001).

In the equilibrium case the thermal conductivity coefficient is obtained by the Fourier transformation of the average equilibrium thermal current autocorrelation function in the limit of zero frequencies, (Allen and Tildesley, 1987; Hansen and McDonald, 1976) as can be seen in the Eq. (7) below, which is commonly named Green-Kubo relation,

$$\kappa = \frac{1}{Vk_bT^2} \lim_{\omega \to 0} \left[ \int e^{i\omega t} \left\langle \vec{J}_x(0) \cdot \vec{J}_x(t) \right\rangle dt \right]$$
(7)

where  $k_b$  is the Boltzmann constant, T is the system temperature and V is the system volume.

The *x* component of the heat current vector is given by

$$J_x(t) = \sum_{i=1}^{N} v_{xi} \varepsilon_i + \sum_{i=1}^{N} \sum_{j=1+1}^{N} v_{xi} (\vec{F}_{ij} \cdot \vec{r}_{ij})$$
(8)

where

$$\varepsilon_i = \frac{1}{2}m_i v_{i^2} + \sum_{j=1}^n u_{ij}.$$
(9)

To obtain a good convergence for the average heat current autocorrelation functions it is necessary a large number of time steps, once the sampling time interval needs to be long enough to avoid any finite time effect, and a high number of samples is desirable to minimize statistical error.

We performed equilibrium simulations in a cubic system, with 5 unit cells side, totalizing 1000 particles, and periodic boundary conditions in all directions. At a constant temperature the average thermal current autocorrelation function was



Figure 8: Thermal coefficient calculated as a Fourier transform of the current-current correlation function (Eq. 7) calculated at T=300K.



Figure 9: Thermal conductivity (blue dots) as a function of temperature calculated from equilibrium molecular dynamics simulation. Red line (Busch & Steigmeier, 1961) and open triangles (Magomedov & Bilalov, 2001) represent the experimental values.

calculated for a 20000 time steps sampling interval. The average was made over 1500 samples in a  $3.10^7$  time steps long run. Each time step represents 1.5fs, so the time interval used for the thermal current correlation function was 30ps. It was verified that this time interval was long enough to stabilize the average calculation, minimizing finite time effects.

Once the average function was obtained, its Fourier transformation was calculated (Eq. 7), in the limit of zero frequencies, to obtain the thermal conductivity coefficient. This procedure was repeated for five different temperatures, 300K, 400K, 500K, 900K and 1000K.

In the equilibrium simulations it can be seen that the sampling time interval chosen for the heat current autocorrelation function calculation was long enough to avoid any finite time effect. In the Fig. 7 it is clear that for a time about 15ps the average autocorrelation function reaches a stable regime. For higher temperatures (data not shown) the stabilization occurs for even smaller times.

The Fourier transform of the autocorrelation function is shown in Fig. 8 and in the limit of zero frequencies it gives a value about  $10Wm^{-1}K^{-1}$  for the thermal conductivity coefficient, which is in a reasonable agreement with experimental value reported by Busch and Steigmeier (Busch and Steigmeier, 1961) and Magomedov and Bilalov (Magomedov and Bilalov, 2001). Figure 9 display the calculated thermal coefficient (filled squares) as a function of temperature along with experimental values reported by these authors. Very good agreement is observed.

### 5 Conclusions

In summary, with the new parametrization for InSb we performed a NPT molecular dynamics simulation to study its pressure-induced transformation and the thermal conductivity. At zero pressure the vibrational density of states is correctly described and when applying hydrostatic pressure two first order transitions were observed: ZB to RS and to CsCl structures. The transition and the equation of state were correctly obtained, in very good agreement with experiments. Although the CsCl phase have been proposed as a final high pressure structure, it was not yet observed experimentally. Studies in nanorods have shown evidences of unusual structures (Yousuf *et al.*, 2003). The interatomic potential proposed is very transferable and could be suitable to explore this new phases. The thermal conductivity as a function of temperature, obtained through the Green-Kubo formula, is also in good agreement with experimental results.

Acknowledgement: We gratefully acknowledge financial support from Fundação de Amparo à Pesquisa do Estado de São Paulo – FAPESP, Conselho Nacional de Desenvolvimento Científico e Tecnológico – CNPq, and Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - CAPES

## References

**Allen, M. P. ; Tildesley, D. J.** (1987): *Computer simulation of liquids*. Oxford University Press, Clarendon.

**Baranyai**, A. (1996): Heat flow studies for large temperature gradients by molecular dynamics simulation. *Phys. Rev. E*, vol. 54, pp.6911-6917.

**Baranyai**, A. (2000): Temperature of nonequilibrium steady-state systems. *Phys. Rev.E*, vol. 62, pp.5989-5997.

**Baranyai**, A. (2001): On the structure and thermodynamics of heat flow in fluids: A molecular dynamics study. *J. Chem. Phys.*, vol. 115, pp.4156-4160.

**Bilz, H. ; Kress, W.** (1979): *Phonon dispersion relations in insulators*. Berlin ; New York: Springer-Verlag.

**Branicio, P. S.; Kalia, R. K.; Nakano, A.; Rino, J. P.; Shimojo, F.; Vashishta, P.** (2003): Structural, mechanical, and vibrational properties of Ga1-xInxAs alloys: A molecular dynamics study. *Appl. Phys. Lett.*, vol. 82, pp.1057-1059.

**Brenner, D.** (2000): The Art and Science of an Analytic Potential. *Phys. Stat. Sol. B*, vol. 217, pp.23-40.

**Busch, G. ; Steigmeier, E.** (1961): Wärmeleitfähigkeit, elektrische Leitfähigkeit, Hall-Effekt und Thermospannung von InSb. *Helv. Phys. Acta*, vol. 34, pp.1-28.

Cahill, D. G.; Ford, W. K.; Goodson, K. E.; Mahan, G. D.; Majumdar, A.; Maris, H. J.; Merlin, R.; Phillpot, S. R. (2003): Nanoscale thermal transport. *J. Appl. Phys.* vol. 93, pp.793-818.

**Chakrabarty, A. ; Cagin, T.** (2008): Computational studies on mechanical and thermal properties of carbon nanotube based nanostructures. *CMC: Computers Materials & Continua*, vol 7, pp.167-189.

Chatterjee, A.; Kalia, R. K.; Nakano, A.; Omeltchenko, A.; Tsuruta, K.; Vashishta, P.; Loong, C. K.; Winterer, M.; Klein, S. (2000): Sintering, structure, and mechanical properties of nanophase SiC: A molecular-dynamics and neutron scattering study. *Appl.Phys. Lett.* vol. 77, pp.1132-1134.

Chiang, K. N.; Chou, C. Y.; Wu, C. J.; Huang, C. J.; Yew, M. C. (2008): Analytical Solution for Estimation of Temperature-Dependent Material Properties of Metals Using Modified Morse Potential. *CMES: Computer Modeling in Engineering & Sciences*, vol. 37, pp.85-96.

**Costa, S. C.; Pizani, P. S.; Rino, J. P.** (2002): Structural phase transformation in InSb: A molecular dynamics simulation. *Phys. Rev. B*, vol. 66, pp.214111.

Costa, S. C.; Pizani, P. S.; Rino, J. P. (2003): Molecular dynamics simulation of dynamical properties of InSb. *Phys. Rev. B*, vol. 68, pp.073204.

Ebbsjo, I.; Kalia, R. K.; Nakano, A.; Rino, J. P.; Vashishta, P. (2000): Topology of amorphous gallium arsenide on intermediate length scales: A molecular dynamics study. *J. Appl. Phys.*, vol. 87, pp.7708-7711.

Erkoç, S. (1997): Empirical many-body potential energy function used in computer simulations of condensed matter properties. *Phys. Rep.*, vol. 278, pp.79-105.

Hansen, J. P.; McDonald, I. R. (1976): *Theory of simple liquids*. London; New York: Academic Press.

**Harrison, W. A.** (1980): *Electronic structure and the properties of solids: the physics of the chemical bond.* San Francisco, W.H. Freeman and Company.

Huang, M. J.; Tsai, T. C.; Liu, L. C.; Jeng, M.; Yang, C. C. (2009): A fast Monte-Carlo Solver for Phonon Transport in Nanostructured Semiconductors. *CMES: Computer Modeling in Engineering & Sciences*, vol. 42, pp.107-129.

**Kubo, R.** (1957): Statistical-Mechanical Theory of Irreversible Processes .1. General Theory and Simple Applications to Magnetic and Conduction Problems. *J. Phys. Soc. Japan*, vol. 12, pp.570-586.

Kunc, K.; Balkanski, M.; Nusimovici, M. A. (1975): Lattice-Dynamics of Several Anb8-N Compounds Having Zincblende Structure .2. Numerical-Calculations. *Phys. Stat. Sol. B*, vol. 72, pp.229-248.

Madelung, O.; Schulz, M.; Weiss, H. (1982): Numerical Data and Functional

Relationships in Science and Technology. In *Landolt-Bornstein, New Series, Group III*: Springer-Verlag, Berlin.

**Magomedov, Y. B.; Bilalov, A. R.** (2001): Thermal Conductivity and the Wiedemann– Franz Relation in Melts of Indium and Gallium Antimonides. *Semicond.*, vol. 35, pp.499-501.

Mujica, A.; Rubio, A.; Munoz, A.; Needs, R. J. (2003): High-pressure phases of group-IV, III-V, and II-VI compounds. *Rev. Mod. Phys.*, vol. 75, pp.863-912.

Nakano, A.; Kalia, R. K.; Vashishta, P. (1994): 1st Sharp Diffraction Peak and Intermediate-Range Order in Amorphous Silica - Finite-Size Effects in Molecular-Dynamics Simulations. *J. Non-Cryst. Sol.*, vol 171, pp.157-163.

Price, D. L.; Rowe, J. M.; Nicklow, R. M. (1971): Lattice Dynamics of Grey Tin and Indium Antimonide. *Phys. Rev. B*, vol. 3, pp.1268-1279.

Rino, J. P.; Chatterjee, A.; Ebbsjo, I.; Kalia, R. K.; Nakano, A.; Shimojo, F.; Vashishta, P. (2002): Pressure-induced structural transformation in GaAs: A molecular-dynamics study. *Phys. Rev. B*, vol. 65, pp.195206.

Schelling, P. K.; Phillpot, S. R.; Keblinski, P. (2002): Comparison of atomiclevel simulation methods for computing thermal conductivity. *Phys. Rev. B*, vol. 65, pp.144306.

Shimojo, F.; Ebbsjo, I.; Kalia, R. K.; Nakano, A.; Rino, J. P.; Vashishta, P. (2000): Molecular dynamics simulation of structural transformation in silicon carbide under pressure. *Phys. Rev. Lett.*, vol. 84, pp.3338-3341.

Stillinger, F. H.; Weber, T. A. (1985): Computer-Simulation of Local Order in Condensed Phases of Silicon. *Phys. Rev. B*, vol. 31, pp.5262-5271.

**Tersoff, J.** (1988a): New Empirical-Approach for the Structure and Energy of Covalent Systems. *Phys. Rev. B*, vol. 37, pp.6991-7000.

**Tersoff, J.** (1988b): Empirical Interatomic Potential for Silicon with Improved Elastic Properties. *Phys. Rev. B*, vol. 38, pp.9902-9905.

**Tersoff, J.** (1988c): Empirical Interatomic Potential for Carbon, with Applications to Amorphous-Carbon. *Phys. Rev. Lett.*, vol. 61, pp.2879-2882.

Vanderborgh, C. A.; Vohra, Y. K.; Ruoff, A. L. (1989): Structural Phase-Transitions in Insb to 66 Gpa. *Phys. Rev. B*, vol. 40, pp.12450-12456.

Vashishta, P.; Rahman, A. (1978): Ionic Motion in Alpha-Agi. *Phys. Rev. Lett.*, vol. 40, pp.1337-1340.

Vashishta, P.; Kalia, R. K.; Nakano, A.; Rino, J. P. (2008): Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. *J. Appl. Phys.*, vol. 103, pp.083504.

**Yousuf, M.; Qadri, S. B.; Skelton, E. F.** (2003): Evidence for the existence of an unusual structure in the nanorods of InSb. *Appl. Phys. A*, vol. 76, pp.133-137.