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Nano Structural Properties of Bismuth

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Abstract: In the last decade, some low-index surfaces of the group V semimetal bismuth have been studied due to their special geometric and electronic structures which including the effect of the interband transition, spin-orbit interaction, (and perhaps, the ad-, rest-and corner-atoms on their surface) and on the electron-phonon coupling. The surface geometric structure of bismuth is more sensitive to incoming atoms and the reconstructions on the surface respect to the bulk structure. This point causes that the surface shows considerably better metallic behavior than that the bulk. We have thus considered XRD (X-Ray Diffraction) spectrum and the spin-orbit coupling for studying the surface electronic structure of Bi. The obtained results indicate that there are strong splitting phenomena at surface state bands due to the loss of symmetry at the surface.

Key words: Nanomaterial · Nanostructure · XRD and Bismuth

INTRODUCTION

Solid state physics is a term used to describe physics involving solid matter and the phenomena that occur in crystals consisting of millions of atoms. Bismuth has been a favorite material for research in quantum confinement that is quantum size effects. Indeed, for the semimetals, a small group of materials with valence bands crossing the Fermi energy but with such low carrier densities (somewhere around 3×10^{17} Cm^{-3} the carriers also have very small effective masses), for an electron along the trigonal axis (in the rhombo hedral structure), the effective mass is $m = 0.003\ m_o$, that they can hardly be classified as metals. Keep in mind that in addition to bismuth, there are the most other prominent semimetals are the group five elements called, As (arsenic) and Sb (antimony).

The precipitate concentration in the nanostructured bulk material increases rapidly with decreasing precipitate size. Even though the volume of these nanoprecipitates accounts for nanograined bulk material, there is a lot of surface area to scatter short wavelength phonons. Besides increasing the carrier concentration, the nanoprecipitates within almost every grain scatter phonons, especially phonons with mean free paths matched with the precipitate size, thus greatly reducing contributions to the lattice thermal conductivity over the wide range of phonon mean free paths present in these thermoelectric materials.

Although quantitatively identifying different contributions of the nanostructures to the transport properties is not possible at this stage, we believe that the nanostructures and imperfections scatter all phonons with mean free paths from the micron scale down to the atomic scale, thus greatly reducing the thermal conductivity [1-3]. Bismuth-rich interface regions and nanoprecipitates contribute to the hole concentration and may also create interfacial barriers that preferentially scatter electrons, both effects leading to a reduction in the bipolar electronic thermal conductivity. One fact that should be mentioned is that the interface regions and nanoprecipitates in the electrical conductivity while their volume increase for the whole nanograined bulk material.

RESULTS AND DISCUSSION

However, the size of nano crystalline bismuth is so important due screening and the possible formation of charge density waves, in where the strength of the electron-phonon interaction for the surface states of Bi is strongly energy dependent. The scattering within the surface state bands depending on the surface and the particular state can get regular secondary and backscattered electrons (not shown).

The detailed analysis of the nanograined nanostructures of bismuth with using XRD technique is shown in Fig. 1. The analysis of Fig. 1 indicates that

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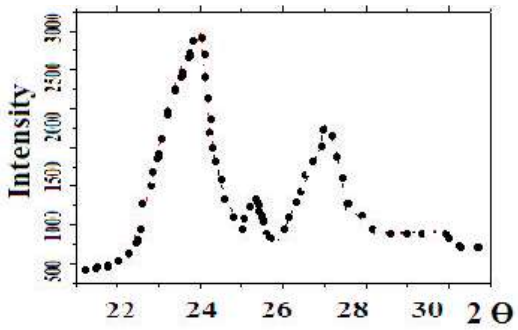

Fig. 1: XRD spectrum of bismuth

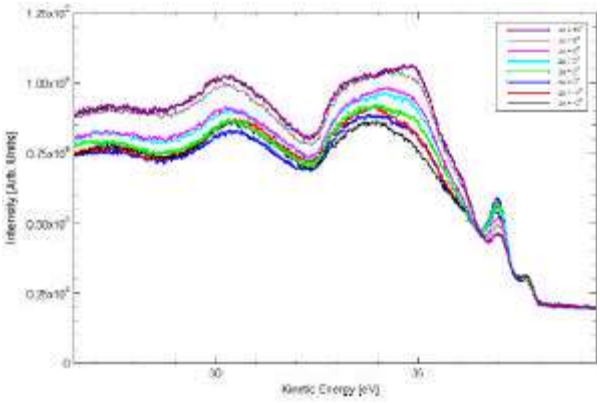

Fig. 2: Angle resolved valence band of the clean silicon substrate

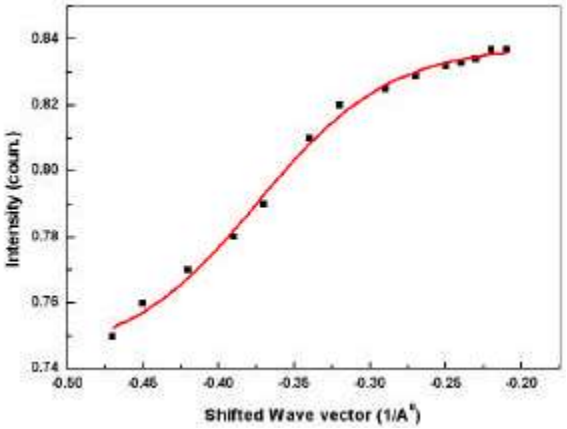

Fig. 3: Intensity versus shifted wave vector

the nanograined bulk material consists of grains, which helps to scatter phonons over the corresponding range of wavelengths and mean free paths. It causes an enhancement of the hole concentration, which leads to an increased electrical conductivity and a reduced bipolar contribution to the electronic thermal conductivity and the Seebeck coefficient. Some workers [1-6] found the stated effects reduce simultaneously the phonon thermal conductivity efficiently.

The most promising of the simple surfaces of Bi are the (100) surface and the (110) surface of this paper, since this surfaces are obtained by breaking covalent bonds, if the surface does not reconstruct the single electron influence the surface electronic structure. Bismuth has an electronic configuration with the filled 5d-shell lying well below the Fermi energy. Recently Ast and Hochst [7] have discussed the origin of this shift and come to the conclusion that the effect is probably not surface induced, but rather associated with inter band losses excited in various parts of the bulk BZ. This has been questioned by Hofmann *et al*. who by different means identify the 5d-band peak as originating from the bulk and surface respectively.

On the one hand, surface states posses several special features. It can only be found in projected band gaps where they do not mix with bulk states. This is easily don for Bi(110). The structure of the (110) surface is assumed to the same as the truncated bulk structure. It consists of double layers separated by nearly the nearest neighbor distance a_{nn}= 3.06 Å. It can escape the crystal without interacting with anything. This is caused by the dispersion of the bulk states which are very much affected by incoming photon energy and the angle between detector respect to normal vector of surface, as revealed in our recent work in [8] and shown in Figure. 2.

Regarding the metallicity of the Bi (110) surface, the most interesting states are cross the Fermi level, states forms a hole pocket creating metallic states effective mass of these states are both estimated to be of the order of one electron mass.

On the other hand, by looking at the shifted wave vector diagram which is obtained analytically and shown in Fig. 3, we are able to identify the effect of structural changing on bismuth properties with regarding to fit obtained data revealed in graph. Similar to what demonstrated in Fig.2, the width (FWHM) of the surface states of bismuth tends to grow for increasing binding energies.

It is also clear that for a surface core level shift, we expect similarly of the states for the 5d-states below the Fermi energy for the $5d_{3/2}$ and $5d_{5/2}$ states [8-14]. The presents of a metallic surface state and thus a change of the density of states (DOS) near the surface of the crystal in the vicinity of the Fermi level is one of the things leading to this effect. This surface core level shift is connected to band narrowing which is large for d-band metals and small for metals whose valence band mainly consist of S and P electrons.

In the present work, we have tried to study the Bi(110) surface in particular, which correspond to the fact that small clusters can be made of bismuth depend inversely with the cluster size. It indicates that the granular systems are related to an enhanced density of states at the Fermi energy provided by surface states, meaning, the Bi (110) surface is indeed metallic with several states present at the Fermi level. This situation can help us to explain the results of the surfaces of bismuth display metallic surface states, which depend on the nature of the cluster surfaces.

CONCLUSION

The obtained results of the present work is basically that Bi (110) surface of is very different from bulk bismuth. Where the bulk has few carriers and low conductivity, the surface appears to be a good metal with an effective mass of the carriers close to that of the free electron mass, which is much higher than that of the bulk carriers. The electronic behavior of a material is closely connected to the geometric structure of that material. Furthermore, the surface structure of bismuth (110) is rather limited. The obtained results indicate that there are strong splitting phenomena at surface state bands due to the loss of symmetry at the surface.

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