Structure and Vibrational Dynamics of Interfacial Sn Layers in Sn/SI Multilayers

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Introduction

Elemental semiconductors with diamond structure, e.g., Si or Ge, are known to exist in amorphous form when prepared either as bulk glasses or as thin films.[1,2] An exception is gray tin (α-Sn), which in the crystalline state is a nonpolar semiconductor with diamond structure and a band gap nearly equal to zero. At ambient pressure, α-Sn is the stable low-temperature phase of bulk tin, which transforms into the metallic body-centered tetragonal β-Sn phase when the temperature is raised above T_c=13.2°C. The α ↔ β phase transition of bulk Sn is an entropy-driven structural transformation that is determined by the difference in vibrational entropy of the two phases.[3]

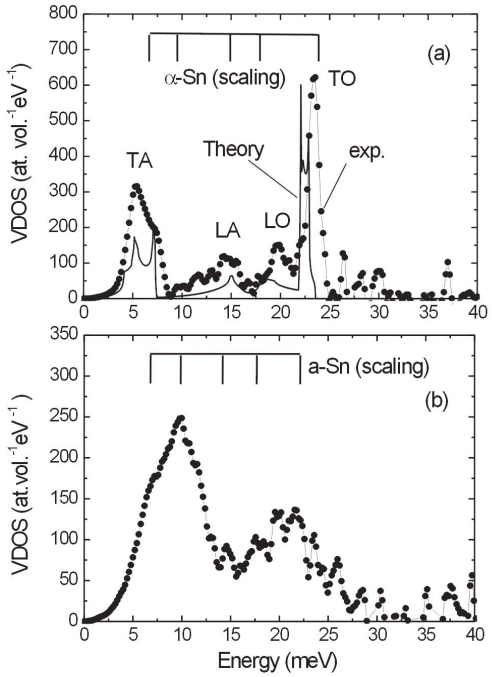

FIG. 1. Vibrational density of states (VDOS): (a) for a-^{119}Sn(500 Å)/InSb(001) (full circles); the theoretical phonon DOS is shown for comparison (bold solid line)[3]; (b) for [^{119}Sn(10 Å)/a-Si(50 Å)]$_{50}$ and [^{119}Sn(10 Å)/a-Si(20 Å)]$_{46}$ multilayers (full circles). The bar diagrams indicate the energies of the prominent peak or shoulder of the various phonon-like bands predicted for amorphous α-like Sn (a-Sn) by scaling.[4]

Methods and Materials

We investigated [^{119}Sn(t_{Sn})/Si(t_{Si})] multilayers of thicknesses t_{Sn}=10, 20 Å and t_{Si} =20, 50 Å. The Sn layers are embedded between amorphous Si (a-Si) layers. The aim of our study was to gain insight on the structure and lattice dynamics of the Sn layers, in particular in the Sn/Si interfacial region. We have employed ^{119}Sn nuclear resonant inelastic x-ray scattering (NRIXS) of synchrotron radiation for the direct measurement of the vibrational density of states (VDOS) of the interfacial thin ^{119}Sn films.

Discussion

By means of NRIXS, we have measured the Sn-projected VDOS in Sn/a-Si multilayers and in 500-Å-thick epitaxial α-Sn on InSb(001) as a reference. The VDOS of the multilayers were found to be distinct from those of the crystalline (bulk) α- and β-Sn phases. Scaling arguments[4] for the VDOS provide further evidence for the amorphous nature of 10-Å-thick α-Sn-like interfaces. Further, the Lamb-Mössbauer factor, the mean kinetic energy per atom, the mean atomic force constant, and the vibrational entropy per atom were obtained (see Fig. 1). The vibrational entropy deduced from the VDOS of a 500-Å-thick epitaxial α-Sn film on InSb(001) is found to be in good agreement with a recent theory[3] At 300K, the observed small difference in vibrational entropy, $\Delta S/k_B$, of + 0.17 ± 0.05 per atom between α-Sn and interfacial amorphous α-like Sn does not account for the stability of the interfacial amorphous Sn layer. Consequently, it is the amorphous-Sn/a-Si interface free energy that stabilizes the metastable amorphous Sn phase. In addition, our results demonstrate that NRIXS is a unique method for investigating the vibrational dynamics of buried interfaces.

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