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Electronic structure and metal-insulator transition in crystalline magnetic phase-change material $Ge_{1-x}Fe_xTe$

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ABSTRACT

X-ray photoemission spectroscopy (XPS) and carrier transport measurements were used to investigate the electronic structure of crystalline $Ge_{1-x}Fe_xTe$ films across the metal-insulator transition. Both valence-band XPS analysis and transport properties indicate that the Fermi energy is shifted downward with increasing Fe concentration. This shift is ascribed to that the incorporated Fe atoms give rise to shallow states near the Fermi energy. Temperature-dependent resistivity measurements reveal that $Ge_{1-x}Fe_xTe$ films undergo a transition from insulating to metallic state at Fe concentration x above 0.1. This metal-insulator transition is attributed to disorder-induced Anderson localization.

1. Introduction

Chalcogenide phase-change materials (PCMs) are of tremendous technological importance since they exhibit fast and reversible transitions between amorphous and crystalline phase [1–3]. These two phases show remarkably different optical and electrical properties, making PCMs currently utilized in non-volatile memory technology. Recently, magnetic phase-change materials were synthesized by doping PCMs with transition metal (TM) elements [4,5]. The magnetic properties, as well as optical and electrical properties, could be conveniently controlled by the phase change feature [4,5]. This new kind of system exhibits potential for multilevel storage owing to the introduction of a new degree of freedom.

In crystalline materials, carrier transport properties are determined by the electronic structure, particularly the band structure near the Fermi energy (E_F) [6]. Understanding and tuning charge transport in crystalline solid is of great importance due to its relevance to practical applications [7]. As for phase-change materials, electronic structure and free-carrier transport properties are investigated in both theory and experiment [7–11]. Recently, a metal-insulator transition (MIT) was observed in crystalline PCM $GeSb_2Te_4$, which provides possibility to enable multilevel resistance states without a change in crystallographic phase [11].

In previous work, we observed a large magnetization contrast between the amorphous and crystalline $Ge_{1-x}Fe_xTe$ films [5]. As a magnetic phase-change material, $Ge_{1-x}Fe_xTe$ is attractive due to its relatively high Curie temperature [5,12,13]. While $Ge_{1-x}Fe_xTe$ films show considerable promise as a candidate material for phase-change memory, the electronic structure and metal-insulator transition behavior have never been investigated. In pure phase-change material GeTe, germanium vacancy leads to empty states at the top of the valence band, thus resulting in p-type conduction [8,9]. As for the TM-doped GeTe, previous calculations indicated that the transition metal dopant plays an important role in the electronic structure [9,10]. Thus, a detailed experimental investigation is required for an understanding of the electronic structure and charge transport in magnetic PCM $Ge_{1-x}Fe_xTe$.

In this letter, we measured the XPS spectra and transport properties of crystalline magnetic PCM $Ge_{1-x}Fe_xTe$. Both valence-band XPS and transport properties indicate that the Fermi energy is shifted downward with increasing Fe concentration. The $Ge_{1-x}Fe_xTe$ films undergo a disorder-induced Anderson metal-insulator transition at Fe concentration x above 0.1, where the Fermi energy exceeds the mobility edge (E_m). The metal-insulator transition was achieved in crystalline magnetic PCM $Ge_{1-x}Fe_xTe$ without a phase change. This detailed investigation gives an insight into the

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electronic structure of $Ge_{1-x}Fe_xTe$.

2. Experimental

$Ge_{1-x}Fe_xTe$ thin films with $x = 0$, 0.02, 0.08, 0.10, 0.14, and 0.25 were deposited on Si (001) substrates by pulsed laser deposition (PLD). The $Ge_{1-x}Fe_xTe$ targets were ablated using KrF excimer laser (Lambda Physik 205 with a wavelength of 248 nm). All the samples were grown at substrate temperature of 300 °C and no annealing process was used. Details of the growth were described in a previous publication [5]. X-ray diffraction and transmission electron microscopy analyses indicated that the $Ge_{1-x}Fe_xTe$ thin films were polycrystalline with rhombohedral structure. The $Ge_{1-x}Fe_xTe$ films exhibit ferromagnetic behavior with a Curie temperature of around 160 K [5]. XPS with a monochromated Al Kα (1486.8 eV) radiation at a pass energy of 50 eV was applied to analyze the electronic structure of $Ge_{1-x}Fe_xTe$ films. The XPS spectra were charge corrected to the adventitious C 1*s* peak at binding energy 284.5 eV. XPS in-depth profile analysis was carried out using an in-situ Ar^+ ion sputtering gun with a sputtering rate of ~10 nm/min, as determined from measurement in the $Ge_{0.92}Fe_{0.08}Te$ film calibrated with a profilometer. Transport behaviors of the thin films were measured in a Van der Pauw configuration.

3. Results and discussions

3.1. X-ray photoemission spectroscopy study

X-ray photoemission spectroscopy is an effective tool for investigating the electronic structures of film materials due to its high surface sensitivity. We measured the XPS spectra of $Ge_{1-x}Fe_xTe$ films after removal of the native oxides by means of Ar^+ ion

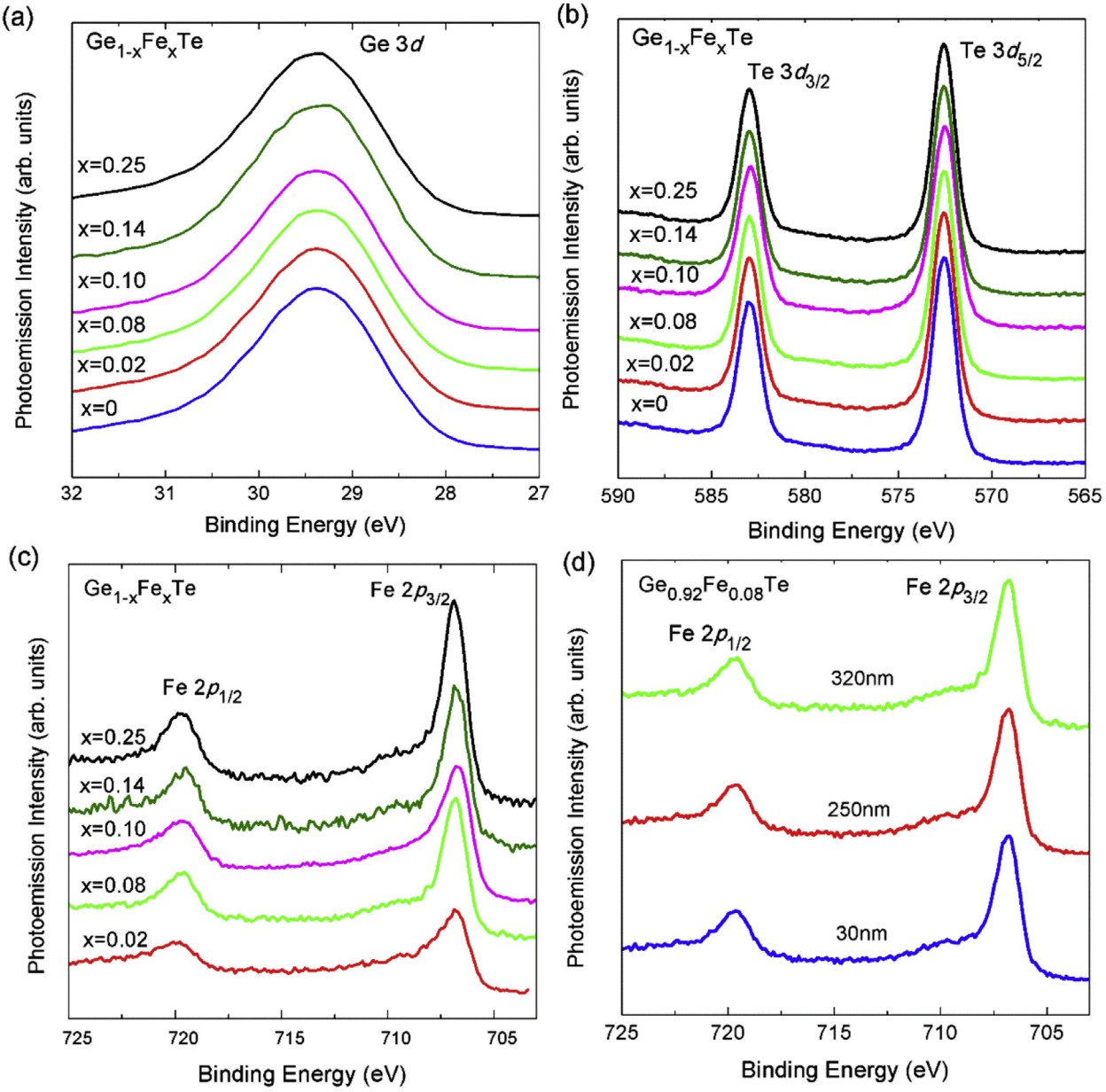

Fig. 1. The Ge 3*d* (a), Te 3*d* (b), and Fe 2*p* (c) core-level XPS spectra in the $Ge_{1-x}Fe_xTe$ ($x = 0$–0.25) films. (d) The Fe 2*p* core-level XPS spectra in the $Ge_{0.92}Fe_{0.08}Te$ film at different depths.