Atomic-scale imaging of local structure of layered Cu-Te phases

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Background incl. aims

Copper-based chalcogenide materials exhibit distinct properties, making them promising candidates for a range of applications [1]. Among these materials, Cu-Te compounds have attracted significant interest due to their versatility in fields like thermoelectricity, memory technology, photothermal therapy, photovoltaics, and batteries. The properties of these alloys are closely linked to their local structure, making accurate description essential for optimizing device performance and advancing material development. The local structure of Cu-Te compounds remains a topic of ongoing discussion [2], especially concerning materials in their low-dimensional form, such as thin films.

This study addresses the controversial aspects of the local structure of Cu-Te phases prepared by thin-film solid-state reaction. Using Cs-corrected scanning transmission electron microscopy (STEM) and atomic-resolution electron energy loss spectroscopy (EELS), the atomic positions of metal and chalcogen atoms in Cu-Te structures are directly visualized. In addition, the investigation revealed the formation of new Cu-Te phase. A crystal structure model for this phase was proposed based on atomic-scale images.

Methods

Atomic-scale investigations are carried out via direct imaging in real space utilizing iDPC, ABF, HAADF and EELS methods. Cu-Te structures are synthesized from metal Cu layer and Sb_2Te_3 epitaxial thin films by thermal heating.

Results

The microstructural investigation of the Cu/Sb2Te3 system unveiled a reaction between the Cu layer and Sb2Te3 upon heating. This reaction led to the formation of van der Waals bonded layered Cu-Te structures, comprising double and triple layers of Te, as depicted in Fig 1. Contrary to existing literature, a detailed analysis of the atomic positions of Cu and quantification of interatomic distances revealed the crystallization of a Cu-rich trigonal Cu1.75Te phase (P-3m1) as the predominant double-layered Cu-Te structure.

Furthermore, a new metastable Cu-rich trigonal phase of Cu1.75Te (P3m1) was found, for which a structural model has been proposed. The phase features a triple-layered structure, resembling the Cu1.75Te double-layered phase. Notably, this metastable phase exhibits vacancies on Cu sites. A detailed analysis of the transition regions suggests that the triple-layered Cu1.75Te structure can easily transformed into the double-layer phase through rearrangements of Cu atoms. Crystal defects, including stacking faults and dislocations, were also observed within the crystal structures. Due to its resemblance to layered Sb_2Te_3 structure, a triple-layered structure was also fabricated as a thin film through solid-state epitaxy of Cu and Sb_2Te_3 layers, using magnetron sputtering at room temperature.

Conclusion

The findings from this study offer valuable insights into the local structure and preferred phases of Cu-Te, which can be relevant during the cycling of Cu-based bulk thermoelectric

materials [3]. This knowledge lays the groundwork for theoretical investigations into their properties and facilitates the design of novel layered materials.

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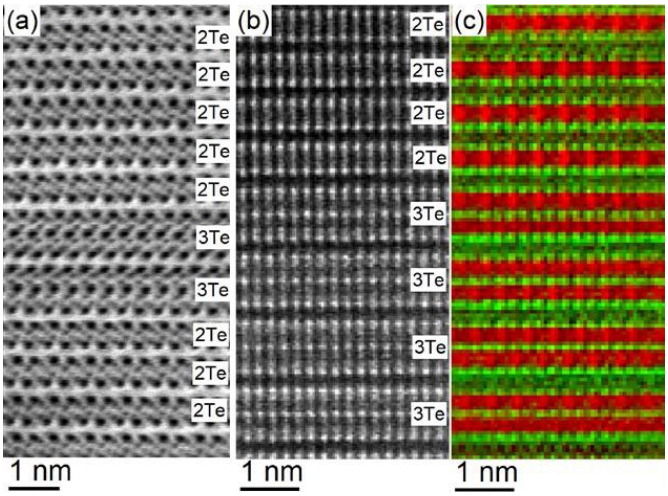
Fig. 1. (a) Atomic-resolution ABF-STEM image showing van der Waals bonded layered Cu1.75Te structures consisting of double (2Te) and triple layers (3Te) of Te. (b) High-resolution HAADF-STEM image and (c) corresponding atomic-resolution EELS maps of Cu (red colour) and Te (green colour).

Graphic:



Keywords:

Thin films, Nanoscale analysis, structure

Reference:

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