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Atom Probe Tomography Analysis of Ag Doping in 2D Layered Material $(PbSe)_5(Bi2Se_3)_3$

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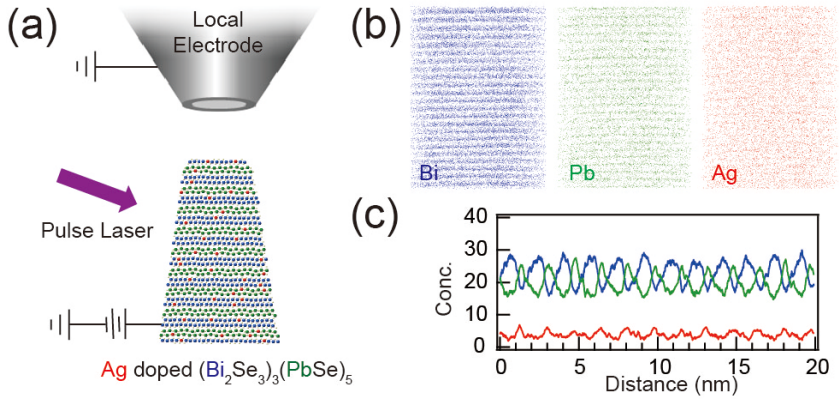

Caption: *(a) Schematic of atom probe tomography measurement. (b) Reconstruction showing the distribution of Bi, Pb and Ag. The layered structure is resolved. (c) 1D concentration profiles of Bi, Pb and Ag.*

Scientific Achievement

The tomographic mapping of dopants in layered 2D materials with atomic sensitivity and subnanometer spatial resolution was achieved for the first time using atom probe tomography (APT) to analyze the Ag dopant distribution in $(PbSe)_5(Bi_2Se_3)_3$. APT analysis shows that Ag atoms are located in both Bi_2Se_3 and PbSe layers in $(PbSe)_5(Bi_2Se_3)_3$, and correlations in the position of Ag atoms suggest a pairing across neighboring Bi_2Se_3 and PbSe layers. Density functional theory (DFT) calculations confirm the favorability of substitutional doping for both Pb and Bi and provide insights into the observed spatial correlations in dopant locations.

Significance

This work proves that APT can resolve the dopant distribution in 2D materials with atomic sensitivity and subnanometer spatial resolution. Thus, APT can play an important role in the development of controlled doping schemes, which is essential for controlling the properties of 2D electronic materials.

First-principles DFT calculations can provide support for an understanding of experimental results and may be further employed to explain the origin of physical properties based on the dopant distribution confirmed by APT. The combination of APT and first-principles calculations has the potential to significantly advance knowledge of structure property relationships at the atomic and nanoscale.

Citation

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