Directional distribution of metal interstitials in Nb2Se3 compound

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Nb_2Se_3 has been known as one of quasi-one-dimensional conductors with chains of metal atoms that occupy a definite site in the structure [1]. This structure-related anisotropic property necessitates direct and simultaneous probing of atomic structure and the relevant chemistry for fundamental understanding of the material behaviour. To this end, we utilized scanning transmission electron microscopy (STEM) with energy dispersive X-ray spectroscopy (EDX) on the atomic level. Observing at different crystal zone axes, we revealed that two geometrically-distinguishable voids (V1 and V2) that are octahedrally-coordinated with Se atoms are distinguished with different volumes and bond distortions in the structure. Intriguingly, we found that Nb atoms preferentially occupy the V1 sites with the largest distorted volume and these Nb interstitials concurrently forms a metal chains along the [010] orientation. Our finding strongly suggests that atomically-aligned Nb interstitial metal chains following the topologically-distinguished one-dimensional void network can contribute to the directional anisotropy in the electrical conduction and quasi-one-dimensional behaviour of Nb_2Se_3 alloy. DFT calculations support that when Nb atoms occupy the V1 sites, the interstitial Nb atoms increase the charge density between inter-layer region of Nb_2Se_3, thus contributing to increasing DC conductivity.

[1] M. H. Rashid and D. J. Sellmyer, Phys. Rev. B 29 (1984) 2359.

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