

Nanoporous structure in titanium silicide cluster by dealloying titanium nickel silicide cluster

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Nanoporous materials have been the focus of much attention due to their huge surface/cavity area in various applications such as catalyst, sensors, and nano-capacitors. An effective method to fabricate nanoporous materials especially nanoporous alloys is *dealloying*, in which a less noble alloying element is selectively dissolved in an aqueous solution. Fukuhara et al. proposed a super capacitor fabricated by dealloying amorphous Si-rich titanium nickel silicide followed by anodic oxidation, where nanoporous titanium oxide with nanometer-sized cavities is observed at the surface region.[1]

In the present work, by means of the first principles calculation (VASP 5.3 with PAW), we investigate nanoporous structure in a titanium silicide cluster, $\text{Ti}_{52}\text{Si}_{100}$ by dealloying a titanium nickel silicide cluster, $\text{Ti}_{52}\text{Ni}_{32}\text{Si}_{100}$. We employ a grain of bulk silicide, $\text{Ti}_4\text{Ni}_4\text{Si}_7$ (tI60, V-phase) as the initial structure. After optimization of the structure of the precursor cluster, Ni atoms in the cluster are removed as a simulation of the dealloying and the structure of the dealloyed cluster is re-optimized. Figure 1 shows the calculated atomic structures of (a) the precursor cluster, $\text{Ti}_{52}\text{Ni}_{32}\text{Si}_{100}$ and (b) the dealloyed cluster, $\text{Ti}_{52}\text{Si}_{100}$. Cavities around Ti atoms are well kept after the dealloying. This structure may suggest experimentally observed titanium oxide with nanometer-sized cavities after anodic oxidation.

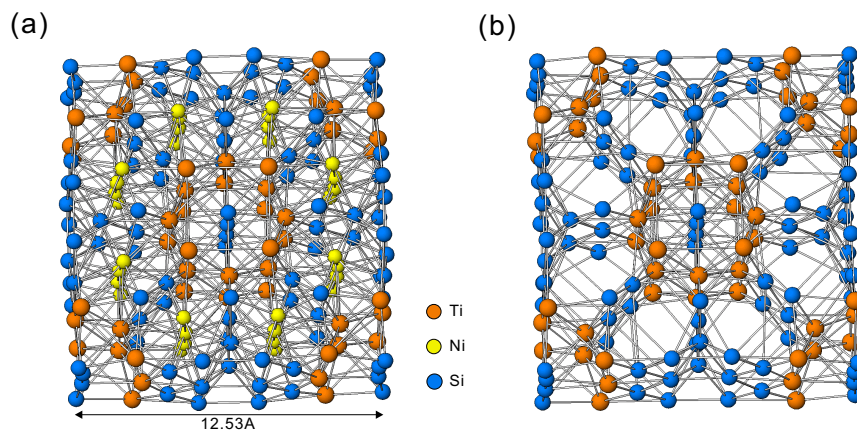


Figure 1: Atomic structures of (a) $\text{Ti}_{52}\text{Ni}_{32}\text{Si}_{100}$ cluster, and (b) dealloyed $\text{Ti}_{52}\text{Si}_{100}$ cluster.

[1] M. Fukuhara, K. Sugawara, *Nanoscale Res. Lett.* 9, 253 (2014).