SUPPLEMENTARY MATERIAL

Softer but tougher: The impact of alloying on defect-free nanoparticles

A. Bisht et al.

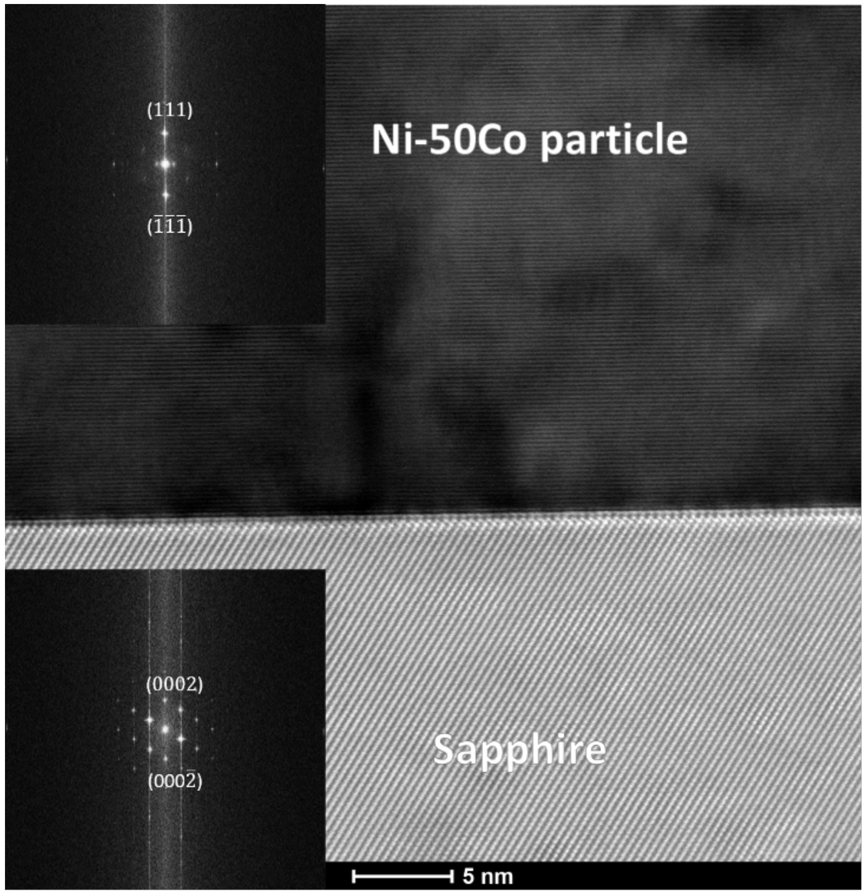

Figure 1: Characterization of the particle-substrate interface. HR-STEM micrograph showing the interface between the Ni-50Co particle and the substrate. The fast-Fourier transform (FFT) confirms that the (111) particle plane is parallel to the (0002) substrate plane and that no intermetallic phases are present at the interface.

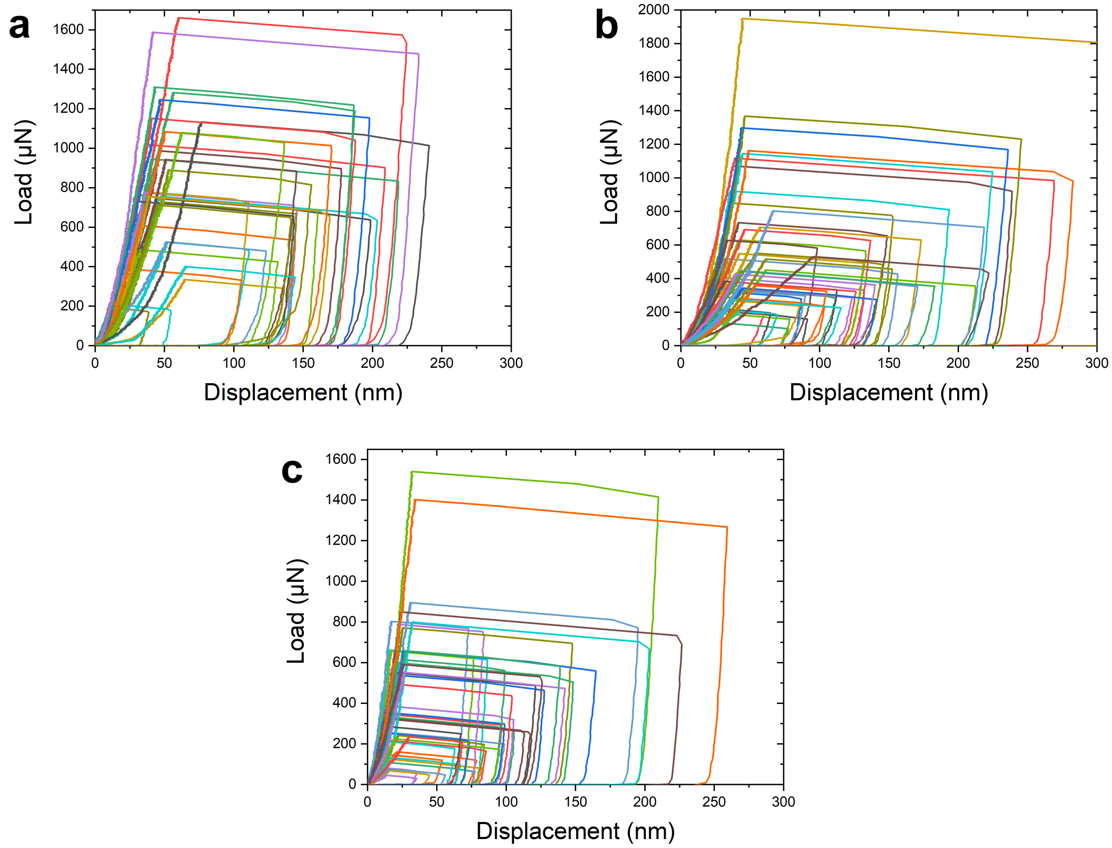

Figure 2: Mechanical testing of nanoparticles. The complete set of load-displacement curves for all particles exhibiting strain burst during compression tests. **a** Ni, **b** Ni-30Co, **c** Ni-50Co

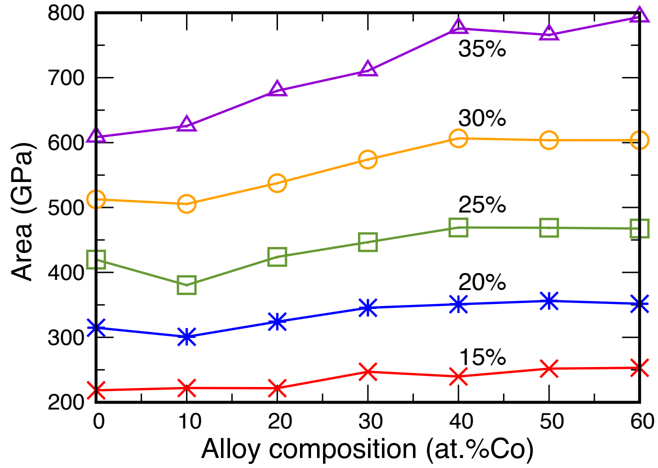

Figure 3: Alloying increases the toughness of nanoparticles. The toughness of 35 nm nanoparticles as a function of chemical composition computed for several stains indicated by the labels.

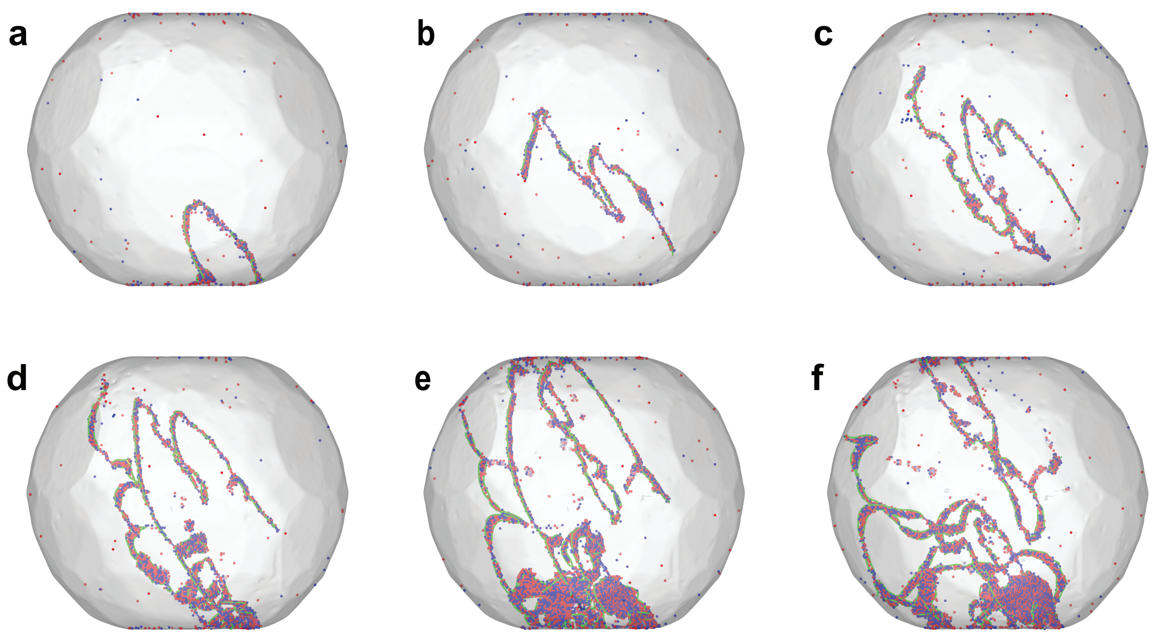

Figure 4: Evolution of dislocation configurations in a 35 nm Ni-50Co nanoparticle. **a**-**d** Sequential snapshots of the particle. **a**-**c** A single dislocation nucleates at the lower facet and propagates deeper into the particle. **d** The dislocation reaches the top and bottom facets, and **e**,**f** causes the nucleation of new dislocations.

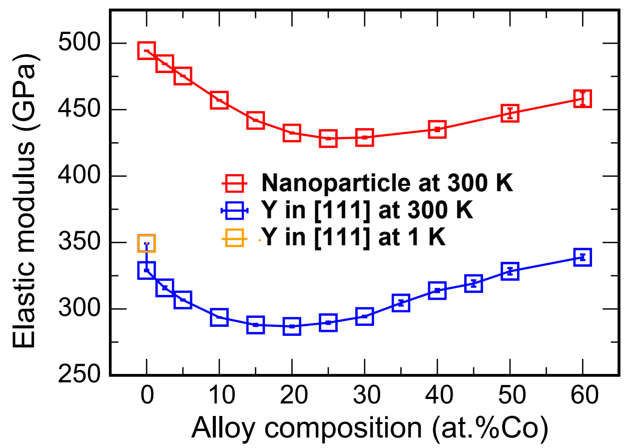

Figure 5: Elastic properties of alloy nanoparticles. Effective elastic modulus of 35 nm nanoparticles as a function of chemical composition compared with the ideal Young modulus $Y_{[111]}$ in the [111] direction at 300 K. The pure Ni Young modulus $Y_{[111]}$ at 1 K is shown as a reference.

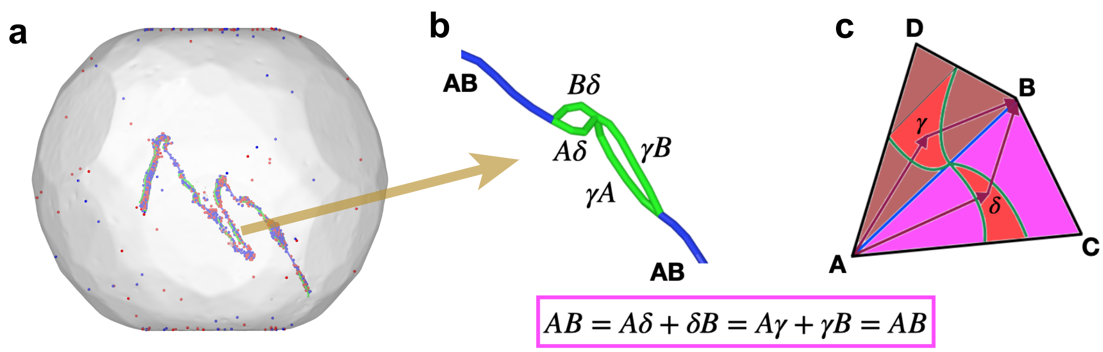

Figure 6: Dislocation cross-slip in Ni-Co nanoparticles. **a** Zigzag-shaped dislocation in a 35 nm Ni-50Co nanoparticle. **b** Dislocation segment of a full dislocation (blue) dissociates into partials (green) in two different slip planes. The visualization is implemented by the DXA algorithm using OVITO [39]. **c** Thompson tetrahedron explaining the crystallography of the cross-slip. The dislocation reaction is shown in the frame.

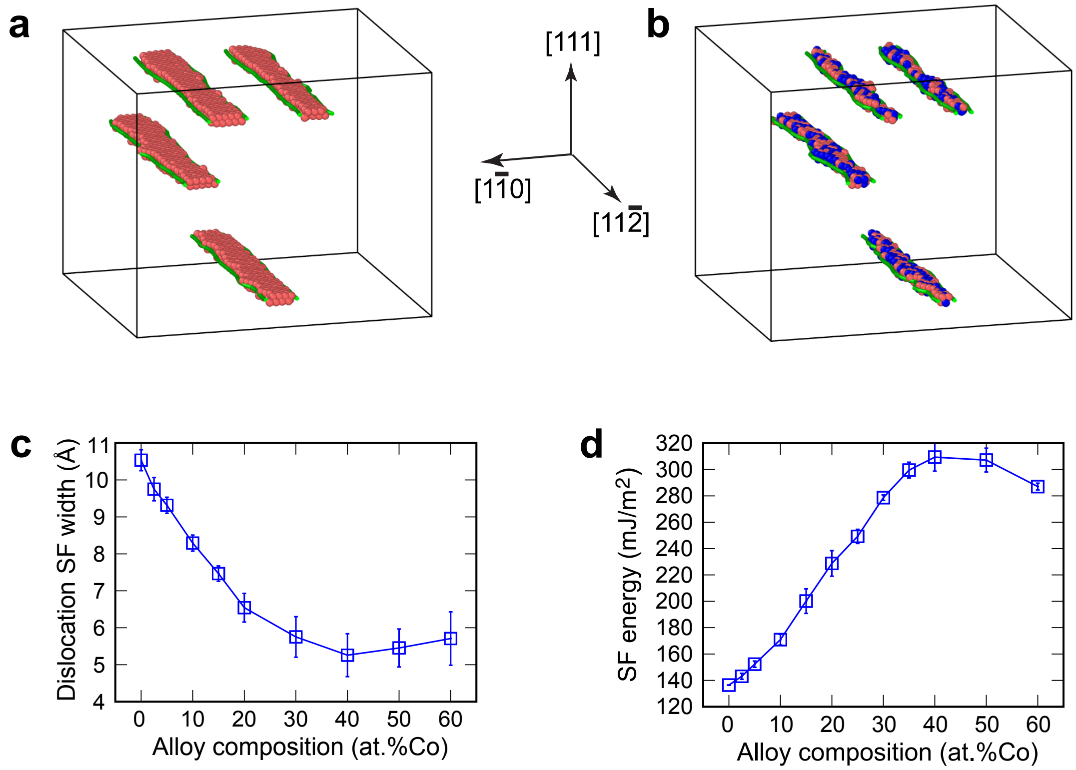

Figure 7: Alloying effect on the stacking fault energy. Edge dislocations in **a** pure Ni and **b** Ni-50Co random alloy. **c** Stacking fault width in the dissociated dislocations as a function of Co concentration. **d** Stacking fault energy as a function of alloy concentration.