## **Supplementary Information**

## On the mechanical response in nanoalloys: the case of Ni-Co

Juan A. de la Rosa Abad<sup>1</sup>, Eduardo M. Bringa<sup>2</sup>, Sergio J. Mejía-Rosales<sup>3</sup> and Marcelo M. Mariscal<sup>1</sup>

<sup>1</sup> INFIQC, CONICET, Departamento de Química Teórica y Computacional, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Córdoba 5000, Argentina.
<sup>2</sup> CONICET and Facultad de Ingeniería, Universidad de Mendoza, Mendoza 5500, Argentina; Centro de Nanotecnología Aplicada, Facultad de Ciencias, Universidad Mayor, Santiago 8580745, Chile.
<sup>3</sup> Centro de Investigación en Ciencias Físico-Matemáticas (CICFIM), Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, Nuevo León 66455, México.

The Supplementary Information includes Figures S1-S8.



**Figure S1.** (a) Dislocation density and force-strain curve of core-shell  $Ni_{12.5}Co_{87.5}$  Snapshots taken at: (b) 6.65%, (c) 7.92%, (d) 8.1%, and (e) 8.71% of longitudinal strain. Shockley partial, Hirth, and Other dislocation are represented by a green, yellow, and red lines, respectively; Co hcp atoms are represented by pink spheres, whereas Ni hcp atoms are represented by green spheres, while fcc atoms are omitted for clarity.



**Figure S2.** (a) Dislocation density and force-strain curve of core-shell  $Ni_{25}Co_{75}$  Snapshots taken at: (b) 5.53%, (c) 7.45%, (d) 7.62%, and (e) 8.66% of longitudinal strain. Shockley partial, Hirth, and Other dislocation are represented by a green, yellow, and red lines, respectively; Co hcp atoms are represented by pink spheres, whereas Ni hcp atoms are represented by green spheres, while fcc atoms are omitted for clarity.



**Figure S3.** (a) Dislocation density and force-strain curve of core-shell  $Co_{12.5}Ni_{87.5}$  Snapshots taken at: (b) 6.18%, (c) 7.63%, (d) 8.54%, and (e) 9.14% of longitudinal strain. Shockley partial, Hirth, and Other dislocation are represented by a green, yellow, and red lines, respectively; Co hcp atoms are represented by pink spheres, whereas Ni hcp atoms are represented by green spheres, while fcc atoms are omitted for clarity.



**Figure S4** (a) Dislocation density and force-strain curve of core-shell  $Co_{25}Ni_{75}$  Snapshots taken at: (b) 5.6%, (c) 6.92%, (d) 7.41%, and (e) 8.81% of longitudinal strain. Shockley partial, Hirth, and Other dislocation are represented by a green, yellow, and red lines, respectively; Co hcp atoms are represented by pink spheres, whereas Ni hcp atoms are represented by green spheres, while fcc atoms are omitted for clarity.



**Figure S5** (a) Dislocation density and force-strain curve of random mix  $Co_{12.5}Ni_{87.5}$ . Snapshots at: (b) 5.15%, (c) 7.01%, (d) 7.67%, and (e) 9.16% of longitudinal strain. Shockley partial, Hirth, and Other dislocation are represented by a green, yellow, and red lines, respectively; Co hcp atoms are represented by pink spheres, whereas Ni hcp atoms are represented by green spheres, while fcc atoms are omitted for clarity.



**Figure S6** (a) Dislocation density and force-strain curve of random mix  $Co_{25}Ni_{75}$ . Snapshots at: (b) 6.0%, (c) 6.3%, (d) 7.0%, and (e) 9.0% of longitudinal strain. Shockley partial, Hirth, and Other dislocation are represented by a green, yellow, and red lines, respectively; Co hcp atoms are represented by pink spheres, whereas Ni hcp atoms are represented by green spheres, while fcc atoms are omitted for clarity.



**Figure S7** (a) Dislocation density and force-strain curve of random mix  $Co_{75}Ni_{25}$ . Snapshots at: (b) 5.0%, (c) 6.41%, (d) 7.0%, and (e) 8.5% of longitudinal strain. Shockley partial, Hirth, and Other dislocation are represented by a green, yellow, and red lines, respectively; Co hcp atoms are represented by pink spheres, whereas Ni hcp atoms are represented by green spheres, while fcc atoms are omitted for clarity.



**Figure S8** (a) Dislocation density and force-strain curve of random mix  $Co_{87.5}Ni_{12.5}$ . Snapshots at: (b) 6.5%, (c) 7.0%, (d) 7.5%, and (e) 8.5% of longitudinal strain. Shockley partial, Hirth, and Other dislocation are represented by a green, yellow, and red lines, respectively; Co hcp atoms are represented by pink spheres, whereas Ni hcp atoms are represented by green spheres, while fcc atoms are omitted for clarity.