Structural shift elucidated with large-scale atomic simulations

July 6 2015

Iron-nickel alloys are ubiquitous: they are found at the earth's core and in meteorites. What is fascinating about such alloys is that their inner structure can change with rapid temperature swings. Heated up above 730 °C (1,340 °F), these alloys enter what is referred to as an austenitic phase. Alternatively, they can be turned into very hard alloys, referred to as a martensitic phase, by subjecting them to extremely rapid cooling. Now a team of scientists from Germany has, for the first time, created a large-scale simulation involving 275,000 atoms representing iron-nickel alloys in proportions found in nature. They show that transitions from one alloy structure to the other occurs in both an orderly and a disorderly way, depending on whether it is heated up or cooled down, respectively. These findings have been published in *EPJ B* by Emilia Sak-Saracino and Herbert Urbassek from the Research Center OPTIMAS at the University of Kaiserslautern, in Germany.

Sak-Saracino showed that using a simulation model makes it possible to uncover morphological changes in iron-nickel crystals occurring as the temperature radically changes. They show that large-scale alloys behave differently than found by previous studies, which focused on samples of the order of thousands of atoms.

Here, the authors show that as the single crystal sample heats up, the alloy's structure changes as a result of the homogeneous nucleation of several grains of poly-crystalline structure, towards an austenitic phase. Conversely, quick cooling of an alloy made of a single crystal type forming a hard alloy proceeds via the heterogeneous nucleation into a

martensitic-style structure. This transformation, they show, requires a larger temperature window for completion than the reverse.

The team also focused on the effect on the alloy structure of the incorporation of nickel into the iron crystal. They show that it lowers the transition temperature necessary to reach the austenitic structure, in agreement with the experimental findings.

More information: "Temperature-induced phase transformation of Fe1-xNix alloys: molecular-dynamics approach," *Eur. Phys. J. B*, DOI: 10.1140/epjb/e2015-60117-x

Provided by Springer