New model should expedite development of temperature-stable nano-alloys

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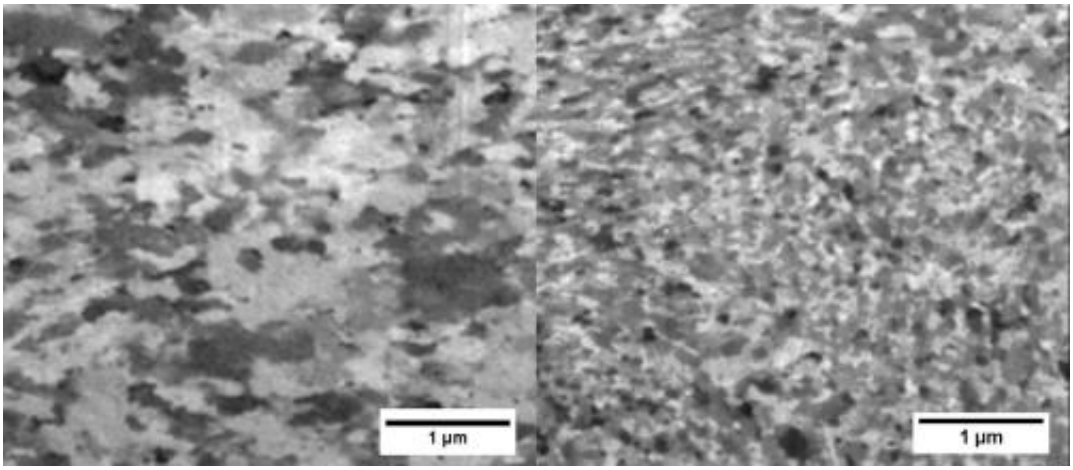

The model correctly predicted the material on the left would not be stable at high temperatures and that the material on the right would retain its nanoscale grain size. The material on the left is Fe-8Ni-4Zr, meaning it is an iron-base alloy with 8 atomic percent nickel and 4 atomic percent zirconium. The grains grew to micron size at 900C. The material on the right is Fe-10Cr-4Zr, meaning it is an iron-base alloy with 10 atomic percent chromium and 4 atomic percent zirconium. This material retained nanoscale grains at 900C. Credit: Mostafa Saber, North Carolina State University

Researchers from North Carolina State University have developed a new theoretical model that will speed the development of new nanomaterial alloys that retain their advantageous properties at elevated temperatures.

Nanoscale materials are made up of tiny crystals, or grains, that are less

than 100 nanometers in diameter. These materials are of interest to researchers, designers and manufacturers because two materials can have the same chemical composition but very different mechanical properties depending on their grain size. For example, materials with nanoscale grains can be harder and stronger than chemically identical materials with larger grains.

But widespread use of nanoscale materials has long been handicapped by the tendency of nanoscale grains to grow when exposed to elevated temperatures – thereby losing their desired mechanical properties.

This is a problem because creating bulk materials from powdered nanomaterials involves exposure to high temperatures, and even nanomaterials made using other techniques may be exposed to elevated temperatures. The grains in some nanomaterials can even grow – and lose their desired properties – when exposed to room temperature for an extended period of time.

A team of NC State researchers decided to tackle the problem by exploring a concept that had been discussed in the research community for some time: stabilizing nanomaterials by introducing small amounts of an additional element. The idea is that this additional element would serve as a stabilizing agent, migrating to the grain boundaries – or interfaces between grains – and preventing the grains from growing at elevated temperatures. Implementing that concept had been daunting, since there are thousands of possible combinations of these elements.

To turn that idea into a practical solution, the researchers developed a theoretical model to identify suitable candidates that can be used as stabilizing agents.

The theoretical model focuses on alloys that consist of two elements, such as iron and chromium, then allows users to see what would happen

if a third element is added to the mix. If users plug the atomic size and thermodynamic properties of each element into the model, the model predicts the grain size of the alloy at any given temperature.

"This model allows anyone to design alloys in a targeted and effective way without having to resort to a trial-and-error approach," says Dr. Ron Scattergood, a professor of materials science and engineering at NC State and senior author of a paper describing the work. "And our experimental results confirm the accuracy of the model."

"We are already using the model in our investigations into lightweight aluminum alloys and high-temperature alloys for nuclear energy applications," says Dr. Mostafa Saber, lead author of the study and a postdoctoral research scholar in materials science and engineering at NC State.

More information: The paper, "A Predictive Model for Thermodynamic Stability of Grain Size in Nanocrystalline Ternary Alloys," was published online Sept. 12 in the *Journal of Applied Physics*. jap.aip.org/resource/1/japiau/v114/i10/p103510_s1

Abstract
This work presents a model for evaluating thermodynamic stabilization of ternary nanocrystalline alloys. It is applicable to alloy systems containing strongly segregating size misfit solutes with a significant enthalpy of elastic strain and/or immiscible solutes with a positive mixing enthalpy. On the basis of a regular solution model, the chemical and elastic strain energy contributions are incorporated into the mixing enthalpy [delta]Hmix, and the mixing entropy [delta]Smix is obtained using the ideal solution approximation. The Gibbs mixing free energy [delta]Gmix is minimized with respect to simultaneous variations in grain size and solute segregation parameters. The Lagrange multiplier method is used to obtain numerical solutions for the minimum

[delta]Gmix corresponding to an equilibrium grain size for given alloy compositions. The numerical solutions will serve as a guideline for choosing solutes and assessing the possibility of thermodynamic stabilization. The temperature dependence of the nanocrystalline grain size and interfacial solute excess can be evaluated for selected ternary systems. Model predictions are presented using available input data for a wide range of solvent-solute combinations. The model predictions are compared to experimental results for Cu-Zn-Zr, Fe-Cr-Zr and Fe-Ni-Zr alloys where thermodynamic stabilization might be effective.

Provided by North Carolina State University