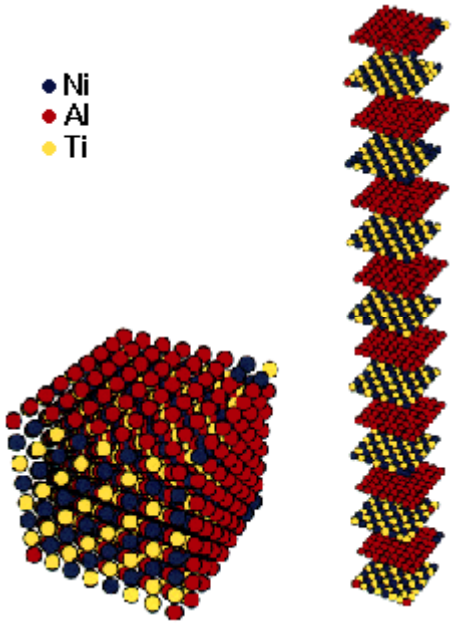
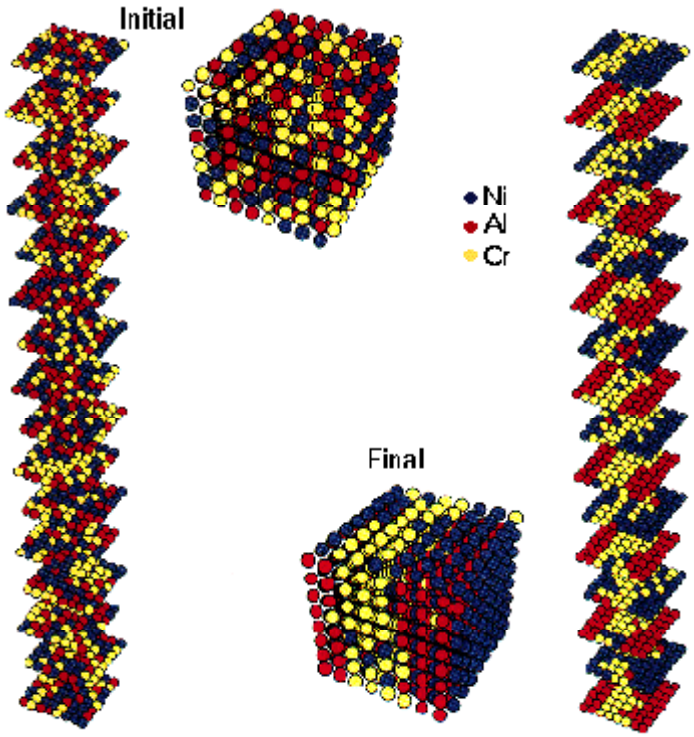
New Theoretical Technique for Alloy Design



$Ni_{50}Al_{25}Ti_{25}$; final temperature, 100 K. (Elongated views, stretched computational cells, are included for the ease of observing these structures.)

During the last 2 years, there has been a breakthrough in alloy design at the NASA Lewis Research Center. A new semi-empirical theoretical technique for alloys, the BFS Theory (Bozzolo, Ferrante, and Smith), has been used to design alloys on a computer. BFS was used, along with Monte Carlo techniques, to predict the phases of ternary alloys of NiAl with Ti or Cr additions. High concentrations of each additive were used to demonstrate the resulting structures.

The computer simulations showed very different behavior for these two alloy systems. NiAl-Ti condensed into the Heusler phase at 25 percent Ti, as shown in the left figure. In contrast, Cr additions resulted in very different behavior predictions (right figure), where we see phase separation of the Cr to regions between the NiAl crystals. Both computations were started at high temperatures with a random distribution of elements that were then Monte Carlo "annealed" to low temperatures, giving the phases shown. These theoretical predictions were verified experimentally by Ronald Noebe et al. Results indicate that it may now be possible to design alloys on a computer, which would greatly aid in narrowing the field of potential alloy candidates for a given application.



$Ni_{33}Al_{34}Cr$. (Elongated views, stretched computational cells, are included for the ease of observing these structures.)

Bibliography

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