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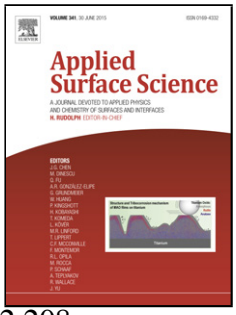

Title: Surface Energy of Metal Alloy Nanoparticles

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Surface Energy of Metal Alloy Nanoparticles

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- **Highlight**
  - Simple equations were used to calculate surface energy of a number of binary metal alloy nanoparticles
  - Binary systems that obey Hume−Rothery rules have close surface energy values that merge at high particle size and form solid solution at macroscopic level
  - Binary systems which are not favorable according to Hume−Rothery rules may form solid solutions at nanoscale.

Abstract

The measurement of surface energy of alloy nanoparticles experimentally is still a challenge therefore theoretical work is necessary to estimate its value. In continuation of our previous work on the calculation of the surface energy of pure metallic nanoparticles we have extended our work to calculate the surface energy of different alloy systems, namely, Co − Ni, Au − Cu, Cu − Al, Cu − Mg and Mo − Cs binary alloys. It is shown that the surface energy of metallic binary alloy decreases with decreasing particle size approaching relatively small values at small sizes. When both metals in the alloy obey the Hume−Rothery rules, the difference in the surface energy is small at the macroscopic as well as in the nano-scale. However when the alloy deviated from these rules the difference in surface energy is large in the macroscopic and in the nano scales. Interestingly when solid solution formation is not possible at the macroscopic scale according to the Hume−Rothery rules, it is shown it may form at the nano-scale. To our knowledge these