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金属纳米微粒晶体结构的稳定性及其结合能

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摘 要： 建立了金属纳米微粒的结合能模型，该模型以微粒尺寸、形状因子和密堆因子为主要参数。根据该模型计算V、Cr、Nb、Mo、Ta、W和Fe元素纳米微粒的结合能。结果表明：一定形状下，在一定的临界尺寸时各纳米微粒bcc结构的结合能和fcc结构的结合能相等；当微粒尺寸大于该临界尺寸时，bcc结构更稳定，小于该尺寸时，fcc结构更稳定。进一步的计算表明，球形和正四面体形可以看作近正多面体形的两个极限，多面体形微粒发生结构转变的临界尺寸介于两个极限尺寸之间，与文献中报道的结果一致。

关键字： 金属纳米微粒；结构稳定性；结合能；形状效应；尺寸效应

Stability of crystal structures of metallic nanoparticles and their cohesive energy

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Abstract: A model was developed to account for the size, shape and structure dependent cohesive energy of metallic nanoparticles. The cohesive energies of V, Cr, Nb, Mo, Ta, W and Fe were calculated. The results show that the cohesive energy of nanoparticles of bcc structure is the same as that of fcc structure at the critical size and specific shape. When the nanoparticle size is larger than the critical size, the nanoparticles in bcc structure are more stable, but when the nanoparticle size is less than the critical value those in fcc structure are more stable. Furthermore, as the nanoparticles is close to the polyhedral shape, the critical size of polyhedral shape lies in the middle of spherical and tetrahedral shape, which is consistent with the experimental and other theoretical predictions.

Key words: metallic nanoparticles; phase stability; cohesive energy; size effect; shape effect

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