

THE SURFACE STRESS AND PHASE DIAGRAMS OF NANOALLOYS DESIGNED FOR LEAD FREE SOLDERS

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Abstract

We have developed the method for calculation of size-dependent phase diagrams, applicable to nanoalloys with variable size of the particles. We have employed combination of CALPHAD method for the modelling of bulk phase diagrams with ab initio calculations of the surface stresses of the constituting elements and relevant intermetallic phases existing in the phase diagram. In this way we have taken into account the surface energy contribution of spherical nanoparticles to the overall Gibbs free energy. In several cases, we studied the variance of surface stress with different crystallographic orientation of the surface. The results have been used for the calculation of phase diagrams of nanoalloys containing Sn, Sb, Ni and Bi, important for the lead free soldering.

Keywords: Surface energy, surface stress, CALPHAD and ab initio modeling of phase diagrams, lead free solders

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