Melting and Glass Transformation of One-Component Systems

Mat.-wiss. u. Werkstofftech. (Materials Science and Engineering Technology) **36** (7), 313-319 (2005)

Hans Juergen Hoffmann

Institute of Materials Science and Technology: Vitreous Materials

Technical University of Berlin

Englische Strasse 20, D-10587 Berlin, Germany

Hoffmann.Glas@TU-Berlin.de

Abstract

Melting of solid chemical elements has recently been explained by electronic transitions. Due to such transitions into higher energy levels the wave-functions and their local charge distributions are changed. Since the occupation of the electronic states and the corresponding charge distribution change at random with time, the core ions are continuously driven to new positions. If the forces are strong enough and the core ions relax to their new positions within the lifetime of the excited states, the changing arrangement of the core ions corresponds to a melt. These considerations are extended from elements to chemical compounds as one-component systems.

The melting entropy and the specific heat capacities near the melting temperature have been normalised to the number of atoms in the formula unit of the one-component systems. The heat capacities exceed $3R$, which is the value expected for vibrations, and accumulate surprisingly at special values as well as the melting entropies. This seems to support the idea of melting as an electronically induced effect.

The distributions of the electronic energy levels in the molten state and in the crystalline solid are different. If the forces of the electronic distribution in the relaxed low energy states of the undercooled melt are too weak to attract the core ions to regular lattice positions, the disorder is frozen-in during cooling and a glass transition takes place. Sufficiently strong directional bonds between neighbouring ions and low melting entropy per particle favour such a transition.

Key words: Melting, melting entropy, specific heat capacity, glass formation, electronic transitions