

Reasons for Melting of Chemical Elements and some Consequences

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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

When studying the causes for melting, solid chemical elements are considered to be the simplest systems. Data of the melting enthalpy, ΔH_m , and entropy, ΔS_m , taken from the literature are investigated as well as the molar specific heat capacities immediately below and above the melting temperature, T_m . In many cases, the molar specific heat capacity at constant volume exceeds the classical limit for the lattice vibrations $C_V = 3R$ above the Debye temperature. This excess specific heat is due to electronic transitions of bonding electrons and of the electrons near the Fermi-edge to states with higher energy. The wave functions of the electrons in these higher states are different from those of the original lower states causing the core ions to be attracted to different new positions. In addition, the vibrations may modify the local potential of the electrons and thus their wave-functions with similar results. Melting occurs if sufficient core ions relax to new positions within the lifetime of the excited states and if their order and arrangement is changing according to the random time series of the different occupied electronic states with their respective wave-functions. This mechanism can also be applied to explain diffusion, thermal expansion and the glass transition temperature.