

## **New Ideas about Melting and the Glass Transition**

Phys. Chem. Glasses **45** (4), 227-237 (2004)

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**

Increasing temperature favours the exchange of electrons from low into higher energy levels. Such transitions are additionally favoured as the energy differences to higher levels in solids decrease due to increasing vibrations of the atoms which modify the local potential. The transitions into higher levels are accompanied by a change of the wave functions and of the local charge distributions. The charge distribution changes according to the random time series of the different occupied electronic states and drives the core ions 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 we have a changing arrangement of the core ions or a melt. The distribution of the electronic energy levels in the molten state differs from that of the crystalline solid. With decreasing temperature the distribution of the electrons relaxes to lower levels of the disordered arrangement. If the forces are too weak to attract the core ions to new regular positions a glass transition takes place. Thus, electronic transitions to higher levels with a sufficiently large deviation of the charge distribution freeze out near the glass transformation temperature and the disorder becomes fixed. This is supported by sufficiently strong directional bonds between neighbouring ions and a low melting entropy.