# Appendix 1.A

## Lindemann criterion

3/01/13



The original Lindemann criterion (Lindemann, 1910) compares the atomic fluctuation amplitude $\langle \Delta r^2 \rangle^{1/2}$ with the lattice constant a of a crystal. If this ratio, which is defined as the disorder parameter $\Delta_L$, reaches a certain value, fluctuations cannot increase without damaging or destroying the crystal lattice. The results of experiments and simulations show that the critical value for $\Delta_L$ for simple solids is in the range of 0.10 to 0.15, relatively independent of the type of substance, the nature of the interaction potential, and the crystal structure (Bilgram 1987; Löwen, 1994; Stillinger 1995). Applications of this criterion to an inhomogeneous finite system like a protein in its native state ('aperiodic crystal', Schrödinger, 1944) requires evaluation of the generalized Lindemann parameter (Stillinger and Stillinger, 1990),

$$\Delta_L = \frac{\sqrt{\sum_i \langle r_i^2 \rangle / N}}{a'} ,$$

where N is the number of atoms and a' the most probable non-bonded near-neighbor distance, $\vec{r}_i$ is the position of atom i, $\Delta r_i^2 = (\vec{r}_i - \langle \vec{r}_i \rangle)^2$, and $\langle\rangle$ denotes configurational

Lindemann, F.A. (1910) The calculation of molecular vibrational frequencies, Physik. Z. 11, 609-612