05.2–31 ATOMIC CONTRIBUTION TO CRYSTALLINE PROPERTY TEMPERATURE DEPENDENCE. By S. C. Abrahams, AT&T Bell Laboratories, Murray Hill, NJ 07974, USA.

Numerous solid state properties are temperature dependent, with major changes in property often occurring at phase transitions. Defining the coefficient of thermal dependence for property X at a temperature T far from a phase transition as $T(X) = (1/X)(dX/dT)$, the average magnitude for many coefficients is on the order of 10^{-3} K^{-1}, with a total magnitude range generally within $\pm$ one or two additional orders. Typical properties in decreasing order of average $T(X)$ include dielectric permittivity, elastic stiffness, piezoelectric strain, magnetic susceptibility, spontaneous strain, spontaneous polarization, piezooptic and linear electrooptic effects, thermal expansion and refractive indices. Assuming distances between covalently bonded atoms are independent of T, the thermal variation of the shortest remaining interatomic distances corresponds to a $T(X)$ of order close to 10^{-3} K^{-1}, within a range of one or two orders of magnitude. A direct relationship is demonstrable between interatomic distance and spontaneous polarization temperature dependence in a number of crystals, and between atomic displacements in ferroelastic transformation and spontaneous strain in several other materials. The thermal dependence of some elastic stiffness coefficients varies inversely both with interatomic distance and with thermal expansion in many compounds, but without common coupling constants. Universal relationships between atomic displacements and resulting physical properties are not to be expected without also considering the electronic contribution. Both are measurable from diffraction experiments: the determination of their temperature dependence in a wide range of materials will provide a sound experimental basis for elucidating the underlying relationships.