International Tables for Crystallography (2006). Vol. D, Section 1.8.6, p. 227.

The peak of the Lorentzian is at ε_0 and the width is γ. Fig. 1.8.5.1 shows the Seebeck coefficient calculated with this functional form. We arbitrarily took $\gamma = k_B T_\gamma$ and $T_\gamma = 100$ K. The four curves are for $\varepsilon_0/k_B = 10, 30, 100$ and 300 K, and the larger ε_0 has the larger Seebeck coefficient. All of the curves have a broad peak as a function of temperature. If $\varepsilon_0 = 0$, then $S = 0$, since the integrand is an odd function of $(\varepsilon - \mu)$. The vertical scale is S/S_0 where $S_0 = k_B/e = 86.17\ \mu\mathrm{V\ K}^{-1}$. We see from Fig. 1.8.5.1 that it is difficult to get values of S/S_0 very much larger than unity.

Another example is that of mixed-valence materials with f electrons. The f shells make electron states of narrow energy, which are approximated as Lorentzians. In this case, $\Sigma(\varepsilon)$ equals the inverse of the right-hand side of (1.8.5.10). The argument for this is that $1/\tau(\varepsilon)$ is proportional to the right-hand side of (1.8.5.10). Since $\Sigma \propto \tau$, it contains the inverse of (1.8.5.10). Interestingly enough, plots of the Seebeck coefficient by Jaccard & Sierro (1982) for this case also contain broad peaks in energy, where S/S_0 has a maximum of about unity. In this case, a proper calculation includes the fact that both C and γ are functions of temperature. For a review, see Mahan (1997).

We give these examples of the Seebeck coefficient because they are the cases that occur most often. In many metals, the Seebeck coefficient is either linear with temperature or has broad peaks. The broad peaks are due to structure in Σ near the chemical potential. This structure is usually due either to variations in the density of states or in the electron lifetime.

In insulators, the Seebeck coefficient can become relatively large. The exact value depends upon the energy gap, the temperature and the density of impurities. This example is treated in many references, *e.g.* Goldsmid (1986) and Rowe (1995).

1.8.6. Glossary

T	temperature (K)
$\mathbf{J}$	current density (A m^{-2})
$\mathbf{J}_Q$	heat current (W m^{-2})
$\boldsymbol{\sigma}$	electrical conductivity (S m^{-1})
ρ	electrical resistivity
K	thermal conductivity (W m^{-1} K^{-1})
$\mathbf{E}$	electric field (V m^{-1})
S	Seebeck coefficient (V K^{-1})
k_B	Boltzmann constant
R_H	Hall constant
m^*	effective mass of the electron
τ	lifetime of the electron

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