

FIG. 5. Plot of $\gamma_e(\delta)$ for K at different temperatures.

of β is in fair agreement with the experimental data; for example, for aluminum we have $\beta = 517$ and $\beta_{\text{exp}} = 500$; for potassium $\beta = 456$ and $\beta_{\text{exp}} = 560$ (β is in erg/g-deg²).

Thus, the Gruneisen coefficient is connected with the character of variation of the density of the electronic states on the Fermi surface, since the value of β is proportional to the density of the electronic states. Usually with increasing density the electronic bands broaden and β decreases, which leads to positive γ_e . A typical example of such a case is Fe (see Table II). The calculated values of γ_e at $\delta = 1-2$ for iron are close to unity, in good agreement with the experimental data. The anomalously large value of β of transition metals is connected with the large density of the electronic states on the Fermi surface for the 3d bands.

In some cases the density of the electronic levels on the Fermi surface can increase upon compression, which leads to a negative γ_e . Such a region of negative γ_e was found in K, as can be seen from Fig. 5. The reason for the appearance of negative γ_e is connected with the fact that at a relative compression 2-3 the hitherto-unfilled 3d

band begins to overlap energetically the 4s band, which leads to an increase of β upon compression, although the width of the fundamental 4s band increases at the same time.

When the temperature increases to $(20-30) \times 10^3$ deg, the calculated value of γ_e reverses sign and becomes approximately equal to 0.15 in the same density interval $2.5 < \delta < 3.5$. The Hugoniot adiabat calculated from this value of γ_e and from the extrapolated section of the cold curve is in reasonable agreement with experiment. At the same time, the large statistical values of γ_e did not permit a noncontradictory interpretation of the

Table II. $\gamma_e(\delta)$ for Fe at different temperatures

T	δ					
	0.746	1.073	2.005	3.00	4.00	5.00
0.004	1.434	1.439	0.953	0.572	0.509	0.397
0.007	1.483	1.387	1.013	0.571	0.507	0.395
0.010	1.607	1.369	1.068	0.566	0.497	0.378
0.020	1.810	1.379	1.032	0.550	0.400	0.240
0.040	1.716	1.386	1.004	0.660	0.388	0.192
0.070	1.462	1.282	1.040	0.810	0.605	0.308
0.100	1.278	1.169	1.189	0.923	0.764	0.449

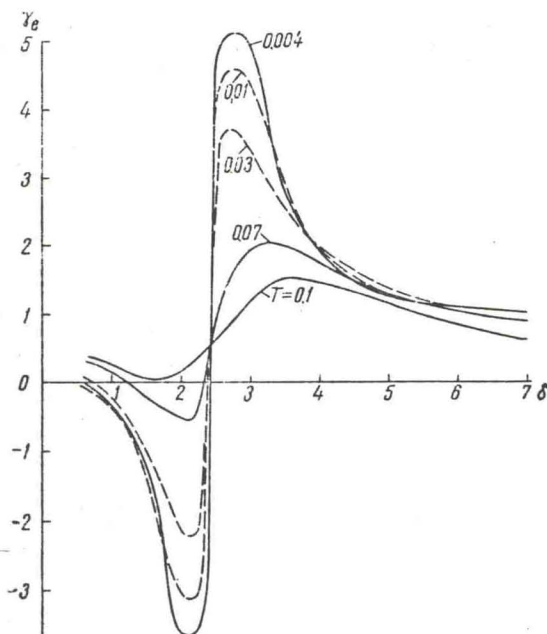


FIG. 6. Plot of $\gamma_e(\delta)$ for aluminum at different temperatures.