GRUNEISEN PARAMETERS AND ISOTHERMAL COMPRESSIBILITY OF GaS SINGLE CRYSTALS

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The temperature dependences of Gruneisen parameters and compressibilities of GaS in the temperature range 80-410K have been investigated. It is shown that the Gruneisen parameters decreases and the compressibilities increases with increasing temperature.

GaS crystallises in the layered structure with hexagonal spatial symmetry D_{6h}^4 and contains four molecular units in the unit cell; lattice parameters at 300 K are a=0.358 nm and c=1.55 nm. Each layer consists of four sublayers in the sequence S-Ga-Ga-S. The bonding between layers is mainly of Van der Waals type, while within layers there exists a strong covalent bond. The weakness of the interlayer bond compared to the intralayer one leads to interesting physical properties, owing to a strong structural anisotropy.

In order to determine Gruneisen parameters and compressibilities we learned elastic properties of GaS. The linear elastic properties may be described with elastic constants. The elastic constants of GaS were calculated from the longitudinal and transverse ultrasound velocities propagating along and perpendicular to the C-axis.

The GaS single crystals were grown by Bridgman technique. The samples were formed in rectangular shape by cleaving and mechanical polishing with dimensions varying 5 to 10 mm along the C-axis, and from 5 to 8 mm in the layer plane. The faces perpendicular to the crystallographic C-axis were easily cleaved reflecting of layered structure. The faces parallel to the C-axis were mechanically polished to make 90±0,5° to the C-face.

The sound velocities were measured by pulse-phase method. From measured velocities and value of the mass density (ρ=3750 kg/m^3) we obtain elastic constants of GaS. At room temperature C_{11}=15,7; C_{13} =1,35; C_{33}=3,87; C_{44}=1,1 and C_{66}=6,15 in units 10^{10} N/m^2. Taking into account the temperature dependence of density the temperature dependence of elastic constants were built [1].

The compressibilities along ($B_{||}$) and perpendicular ($B_{\perp}$) to the C-axis can be expressed in terms of the elastic constants, yielding:

$$B_{||} = \frac{C_{11} + C_{12} - 2C_{13}}{C_{33}(C_{11} + C_{12}) - 2C_{13}^2},$$

$$B_{\perp} = \frac{C_{33} - C_{13}}{C_{33}(C_{11} + C_{12}) - 2C_{13}^2},$$

$$B = B_{||} + 2B_{\perp}.$$

Using the elastic constants, we obtain $B_{||}$≈0,23; $B_{\perp}$≈0,036, B≈0,302 in units 10^{-10} Pa^{-1}. These values are in agreement with calorimetric measurements. Thus, the crystal is much more compressible along the C-axis than perpendicular to it.

The compressibility anisotropy is due to large difference of intra- and interlayer forces.

In the temperature region 80-410 K compressibility linear increase with increasing temperature and the slope of $B_{||}$ more than that of $B_{\perp}$. This fact indicates that along the C-axis contribution of thermal expansion to value of compressibility is much more than perpendicular to it.

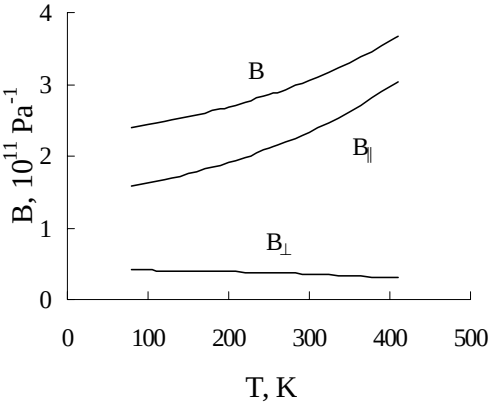

Fig.1. The temperature dependence of isothermal compressibility B of GaS single crystals: $B_{||}$, $B_{\perp}$ - compressibilities along and perpendicular to the C-axis, respectively.

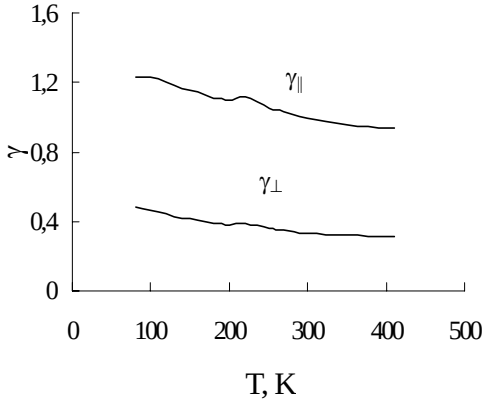

Fig.2. The temperature dependence of Gruneisen parameters of GaS single crystals: $\gamma_{||}$, $\gamma_{\perp}$ - Gruneisen parameters along and perpendicular to the layer plane.

The Gruneisen parameters also can be obtained from

elastic constants. In the case of hexagonal crystals, one can define two independent Gruneisen parameters: $\gamma_{\parallel}$ and $\gamma_{\perp}$. They are related to the elastic constants by

$$\gamma_{||} = \frac{V}{C_P}\left[(C_{11} + C_{12})\alpha_{||} + C_{13}\alpha_{\perp}\right],$$

$$\gamma_{\perp} = \frac{V}{C_P}\left[C_{33}\alpha_{\perp} + 2C_{13}\alpha_{||}\right],$$

where V – molar volume; C_p – molar heat capacity at stationary pressure; α_i – components of the thermal expansion.

In [2] the temperature dependence of Gruneisen parameters was built without taking into account the temperature dependence of elastic constants. According to [2] $\gamma_{\parallel}$ is negative in the narrow temperature interval 30-50 K and this can be understood with a main role ″bending″ waves in thermal properties of layer crystal.

In view of temperature dependences of elastic constants [1], thermal expansion [3] and heat capacity [4] the temperature dependence of Gruneisen parameters were built in the temperature region 80-410 K. At T=200 K our values $\gamma_{\parallel}$=1.073, $\gamma_{\perp}$=0.379 are in a good agreement with data [2]: $\gamma_{\parallel}$=0.8, $\gamma_{\perp}$=0.35. As it is shown, $\gamma_{\parallel} > \gamma_{\perp}$. Thus anharmonicity of the interatomic forces is more in the strong bonding direction.

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GaS MONOKRİSTALLARININ QRUNAYZEN PARAMETRLƏRİ VƏ İZOTERMİKİ SIXILMASI

80-410K temperatur intervalında GaS monokristallarının Qrunayzen parametrlərinin və izotermiki sıxılmasının temperatur asılılıqları tədqiq edilmişdir. Göstərilmişdir ki, temperaturun artması ilə Qrunayzen parametrləri azalır, izotermiki sıxılma isə artır.

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ПАРАМЕТРЫ ГРЮНАЙЗЕНА И ИЗОТЕРМИЧЕСКАЯ СЖИМАЕМОСТЬ МОНОКРИСТАЛЛОВ GaS

Исследованы температурные зависимости параметров Грюнайзена и изотермической сжимаемости монокристаллов GaS в интервале температур 80-410K. Показано, что с увеличением температуры параметры Грюнайзена уменьшаются, а изотермическая сжимаемость увеличивается.

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