

THERMAL AND ELECTRICAL CONDUCTIVITIES OF SILICON IN SOLID AND LIQUID STATES

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Abstract. The thermal and electrical conductivities of silicon have been investigated in solid and liquid states. It is shown that in solid state region at temperatures close to melting point phonon and electron mechanisms including the ambipolar part are dominant in thermal conductivity. The electronic contribution including the ambipolar part was computed from the Wiedemann-Franz and Davidov-Shmushkevich relations for a nondegenerated electron gas and did not exceed 25% from the total thermal conductivity. The deviation in the temperature dependence of phonon thermal conductivity from the T^{-1} law observed at high temperature can be explained in terms of scattering of acoustical phonons by the optical one.

The thermal and electrical conductivities of the Si increase at melting and the magnitude of these parameters becomes close to those one of metallic melts. It is shown that calculated values of the Lorentz number and electrical conductivity in melts of Si unlike those in metals change with temperature after melting. The anomalous temperature dependence of the electrical conductivity and of the Lorentz number at temperatures near the melting point is consistent with anomalous for metallic melts temperature variations in density, viscosity, free energy and entropy of the viscous flow of melts of the silicon in the same temperature range.

Introduction.

Much attention in recent years has been given to the problem of structural disordering and its influence on the kinetic properties of semiconductors and metals. Several models have been proposed to theoretical explanation of the effect of melting on charge transport in semiconductors. The most appropriate explanation appears to be offered by Mott's theoretical model (Mott and Davis 1979). According to this model three types of transformations of the density of energy states of charge carriers in semiconductors are possible depending on the extent of the changes in Short-range order during melting: the transition to the metallic state, the transition to a semimetallic state or the preservation of semiconducting properties. Arranging the melts studied at that time in decreasing order of magnitude of electronic conductivity Allgaier (Allgaier 1969) distinguished three groups of melts A, B, C which correspond to the three types of energy-dependent transformation of electron density of states in Mott's model.

The A group includes among the melts of common metals the melts of semiconductors with electrical conductivity exceed $5 \cdot 10^5 \Omega^{-1}M^{-1}$. The melting of these semiconductors is accompanied by drastic changes in the short-range order and an abrupt changes of electrical conductivity, thermal emf, Hall coefficient and other number of parameters. The magnitudes of all these parameters become close to those in metallic melts. However, the temperature dependence number of these parameter unlike those in metals after melting (Glazov et al, 1969).

A specific feature of the metallic state of a substance is that the major heat and charge carriers in them are free electrons and the Wiedemann-Franz relation between thermal and electrical conductivities.

In metal-like semiconducting melts belonging according to Mott to the A group, the Wiedemann-Franz relation is not studied because of the lack of reliable experimental data on thermal conductivity.

In order to identify the mechanism of thermal conductivity and to verify the validity of the Wiedemann-Franz relation, we studied the thermal and electrical conductivities of silicon at high temperatures in solid and liquid states.

Experiment.

We have studied the thermal conductivity of silicon and its melts by means of the absolute spherical method in stationary thermal regime (Magomedov, 1990). The sample having spherical film shape 2-3 mm thickness is bounded by two concentric pure graphite spheres. Graphite spheres were machined in halves and sealed together with grease produced on the basis of a finely dispersed graphite powder. Six uniformly distributed alumina dowels of 1 mm diameter were screwed into the inner sphere, and served to align the two spheres on assembly. The careful measurements of the individual halves showed that the maximum variation of the radius in any direction was not exceed 0,02 mm. An electric heater consisting of alumina core wrapped with molybdenum resistance wire was cemented into a cavity of the inner graphite sphere. The temperature drop through the test sample was measured with a wolframium-rhenium thermocouples but the heat flow by the electrical power of the heater. The error of the thermal conductivity measurements does not exceed 6% at 1300 K.

The electrical conductivity was studied by the four-probe compensation method (Magomedov et al 2003). The substance under study fills a vertical quartz cell 4-5 mm in diameter and 50-60 mm long with two lateral holes for graphite rods, which have holes drilled in them for thermocouples and potential probes. The top and bottom of the working cell are tightly jointed to graphite caps operating as current leads and additional vessels for the substance. The working cell with the graphite caps and rods is sealed using a grease produced on the basis of a finely dispersed graphite powder. Heaters insulated by a mica plate from the parts of the apparatus, are put on the graphite caps. The heaters produce a uniform temperature field or a certain temperature difference during the conductivity or thermal-emf measurements, respectively. The temperature regime during the measurements is controlled with a regime heater whose operation is controlled by a thermoregulator.

To prevent the oxidation of the substance under study and parts of apparatus and the possible evaporation or decomposition of the investigated compounds at high temperatures, investigation of thermal and electrical conductivities were carried out in an autoclave in an inert-gas atmosphere (argon or helium), with which the autoclave was filled after its evacuation to a pressure of $1.33 \cdot 10^{-2}$ Pa through a branch pipe. The pressure of the inert gas in the autoclave is monitored by a monometer with a valve and is controlled with an allowance for the pressure of the saturation vapors of the elements incorporated into the compound under study. The temperature difference across the samples is measured by WRe 5-WRe 20 thermocouples, which are inserted into alumina tubes and laid into the holes in the graphite rods. The W and Re branches of the thermocouples are used separately as probes for picking of the voltage drop and

potential difference in measurements of the electric conductivity and thermal emf, respectively.

The error of the electrical conductivity measurements does not exceed 4% at 1000K.

Results and discussion.

The experimental results of the temperature dependence of thermal and electrical conductivities of Si and its melts are shown in fig. 1.

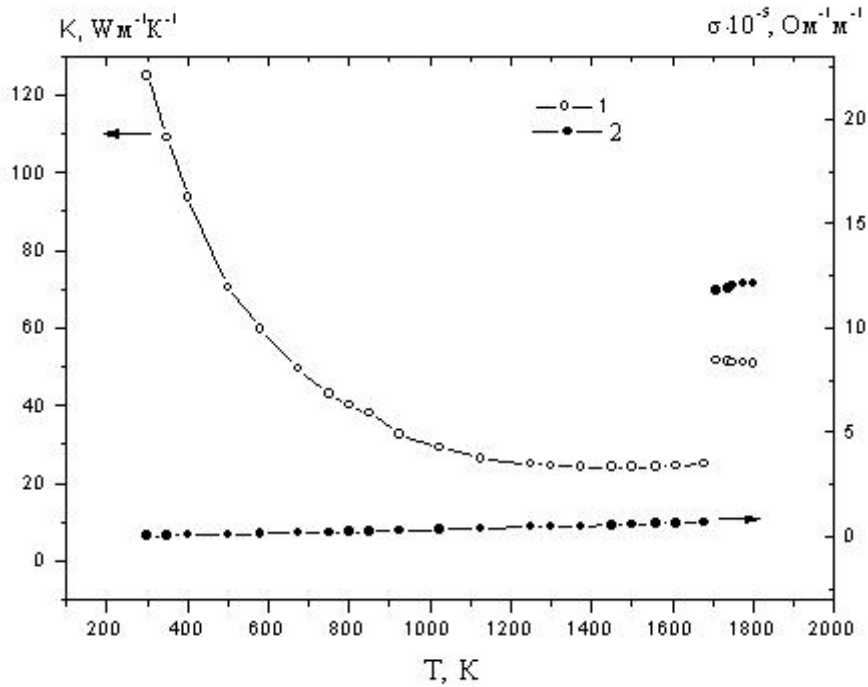


Fig. 1. The temperature dependence of thermal (1) and electrical (2) conductivities of Si and its melts.

It is shown that in solid state region at temperature close to melting point phonon and electron mechanisms including the ambipolar part are dominant in thermal conductivity. The electronic contribution including the ambipolar part was computed from the Wiedemann-Franz and Davidov-Shmushkevich relations using the data on electrical conductivity and thermal emf a nondegenerate electron gas.

The temperature dependence of the phonon thermal conductivity of the Si follows simple T^{-1} law as postulated by Leibfried-Shleman's relationship for 3-phonon process at temperatures below 800°K. The deviation in temperature dependence of phonon thermal conductivity from the T^{-1} law observed at high temperatures can be explained in terms of scattering of acoustical phonons by the optical phonons.

The thermal and electrical conductivities of silicon increase at melting and the magnitude of these parameters becomes close to those of metallic melts. However, the thermal and electrical conductivities in melts of the Si at temperature near the melting point change with temperature (σ increase and λ decrease) unlike those in metals (Filipov 1970).

Using the temperature dependence of heat capacity and density was calculated the molecular thermal conductivity of the melts.

The values of the Lorentz number L for various temperatures were also calculated using the experimental data on thermal and electrical conductivities and taking into account the value of molecular thermal conductivity from the Wiedemann-Franz relation. The value of the Lorentz number ($L=2.5 \cdot 10^{-8} \text{ W}^2/\text{K}^2$) and its temperature dependence (L decrease with temperature in the range of 150K after melting from $2.5 \cdot 10^{-8} \text{ W}^2/\text{K}^2$ to $2.4 \cdot 10^{-8} \text{ W}^2/\text{K}^2$) are not typical for metallic melts. The anomalous value and temperature dependence of the Lorentz number and thermal and electrical conductivities at temperatures near the melting point is consistent with anomalous (for metallic melts) temperature variation in density, viscosity, free energy and entropy of activation of the viscous flow of silicon melts in the same temperature range. The anomalous behaviour of these parameters in the melt of Si is explained by the inherited features of solid state structures in a certain temperature range after melting.

The decrease in the Lorentz number and anomalies in the temperature behavior of other parameters upon further heating of the Si melts suggest that the process of structural transformation and metalisation in melts of the Si is not completed at melting and is fully completed only after overheating by 150-200 K.

In our opinion the melt of Si just after melting have intermediate properties between metal melts and the B group melts according to Mott's classification.

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