

2 Fundamentals of Flash Lamp Annealing of Shallow Boron-Doped Silicon

MSA of semiconductors is usually performed using flash lamps. It has been shown that FLA holds the balance between effective dopant activation and a low diffusion rate into the bulk [8], [9]. Moreover, it allows for thermal processing of surfaces and interfaces independently of the substrate material. Furthermore, in contrast to laser annealing, FLA enables one to perform thermal treatment of large-scale samples without increasing the process time.

2.1 Electrical and Optical Characteristics of Flash Lamps

Figure 1 shows the general set-up of an FLA chamber. A set of halogen lamps preheats the sample back to prevent thermal stresses and shock in the wafer, which may cause breakage due to the temperature gradients occurring as a consequence of the millisecond heating.

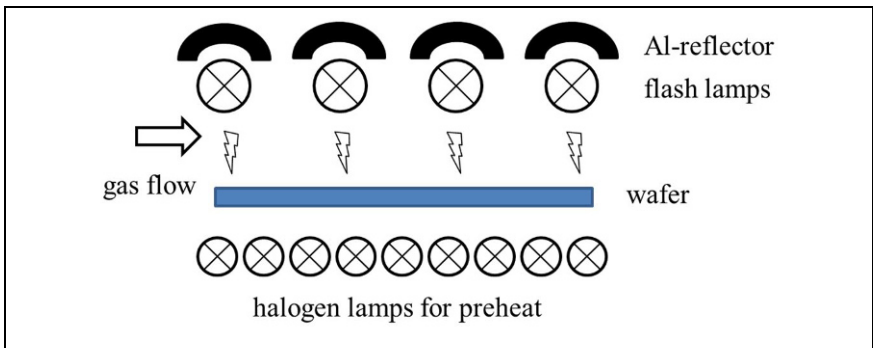


Figure 1: Schematic drawing of the set-up of an FLA apparatus.

The halogen and flash lamps, which are filled typically filled with Xenon or Argon, are protected by a 3 mm thick quartz plate from possible evaporation of gases from the sample. A gas flow – usually of Nitrogen or Argon – ensures an inert atmosphere. Above the flash lamps Aluminium reflectors are mounted to decrease the loss of light intensity for annealing. The round shape of the reflectors is chosen such that the flash light is collimated onto the wafer surface. The flash lamps can be operated between pulse times of

130 μs and 80 ms at full width half maximum (FWHM). The maximum energy density on the surface amounts to approximately 150 J/cm² which is limited by the capacitance of the lamp circuit. The housing of the chamber is made of Aluminium which melts at a temperature T of 933.47 K. However, due to the high reflectivity of Aluminium the flash cannot heat it up to its melting temperature. Still water cooling is supplied to the chamber walls and to the Aluminium reflector during the preheating step.

An LC resonator consisting of coils with inductance L and capacitors with capacitance C creates flash pulses with a time duration $t = \frac{1}{f}$, whereby

$$f = \frac{1}{2\pi\sqrt{LC}}. \quad (1)$$

The electric energy

$$E = \frac{1}{2}CU^2 \quad (2)$$

that is stored in the capacitors can be calculated knowing the capacitance C and the charging voltage U , whereas the discharge of the capacitors is retarded by the presence of the coils as a function of inductance. The optical energy output of the flash lamps is by some factor smaller than the electric energy. This factor is a technical parameter that is characterised by the fill gas, the internal pressure, the glass type envelope and the applied voltage.

With respect to the energy stored in the capacitors, an efficiency of the flash lamps can be defined with regard on the emitted optical output. Theoretically, using Xenon-filled flash lamps an energy efficiency of about 50 % is possible [10]. Figure 2 shows the effective lamp output for two different devices and the flash lamps used for the present thesis. The measurement has been performed by an energy density meter with a wavelength range from 400 nm to 1400 nm. The depicted theory considers the energy stored in the capacitors according to Equation (2) per unit flash lamp area. The differences in the absolute values of energy density for the two chamber devices represent different geometries / lamp bank areas. These results reproduce the theoretical upper limit of 50 %. For flash pulses with time durations of 20 ms and 3 ms at FWHM at a low charging voltage, a significant deviation from this theoretical value cannot be found.

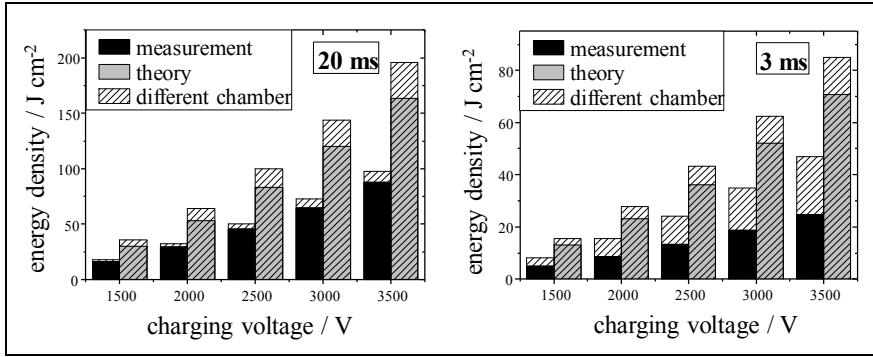


Figure 2: Comparison of the theoretical (predicted by Equation (2)) and measured energy densities for flash pulse times of 20 ms (left) and 3 ms (right) at FWHM.

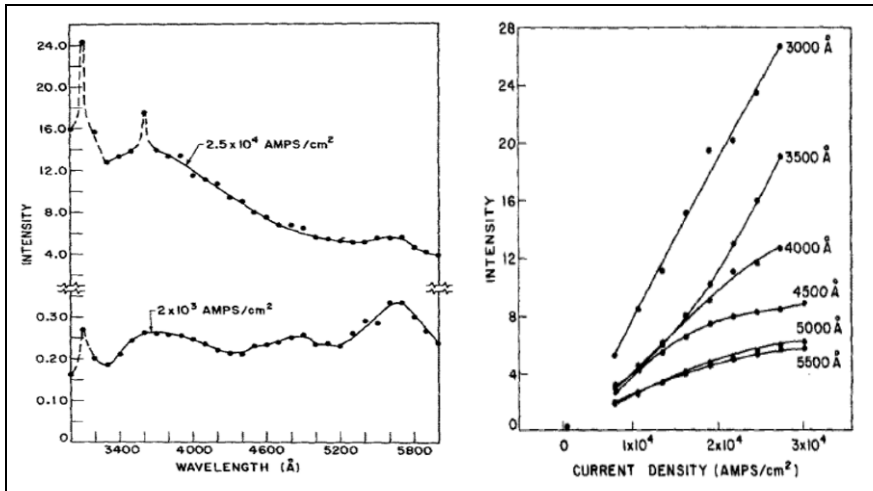


Figure 3: Increase in the UV output of a Xenon-filled flash lamp as a function of wavelength and current density. Left: The Xenon spectrum is shown for two different current densities. Right: Peak position on the wavelength scale and intensity for growing current density (figure taken from [11]).

Due to recombination and collision of free electrons with bound positive Xenon or Argon ions in the high pressure tube, the emission spectrum of the flash lamps is continuous as shown in Figure 3. High current density increases the optical output in the UV/Vis region whereas for low current

density spectral emission lines of the excited Xenon/Argon ions dominate the flash lamp output (cf. Figure 3). The steep rise of peak intensity at a wavelength of 3000 Å for elevated current densities in the right graph of Figure 3 shows that UV output is strongly enhanced for large current densities [11].

2.2 Absorption of Light in Single-Crystal Silicon during Flash Lamp Annealing

According to the spectrum of a Xenon-filled flash lamp in Figure 3 for a material to be suitable for millisecond annealing two prerequisites need to be fulfilled. First, it needs to be absorbing in the visual part of the electromagnetic spectrum and second, the time scale of annealing should be in the order of the light thermal response time [2].

Silicon crystallises in a face-centred cubic structure with a two atom base at $\{(0,0,0) (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})\}$ (diamond structure). Each Silicon atom is the heart of an even tetrahedron with four sp^3 hybrid orbitals stretching out to the corners of a virtual tetrahedron. In the direction of each hybridised orbital there is another sp^3 orbital from a neighbouring Silicon atom to overlap and form a covalent bond. The corresponding band diagram in Figure 4 shows that Silicon is an indirect band gap semiconductor with a bandgap energy at 1.12 eV. However, Silicon also has local direct bandgaps E_{r1} and E_{r2} as shown in Figure 4. E_{so} , E_X and E_L refer to the energy gap due to spin-orbital-splitting and the energy separation between the valence band maximum and the X- and L-valley of the conduction band, respectively.

Indirect transitions require phonon participation to supply the remaining quasi-momentum $\hbar k$. The requirement of phonon participation for optical absorption in an indirect semiconductor decreases its absorptivity $\alpha_0(\lambda)$ as shown in Figure 5. The absorption coefficient at the indirect bandgap E_g is comparatively low with respect to its value at the direct bandgaps E_{r1} and E_{r2} for all temperatures. As a guidance to the eye the absorption spectrum in the vicinity of the indirect band gap is plotted on a logarithmic scale (see inset in Figure 5).

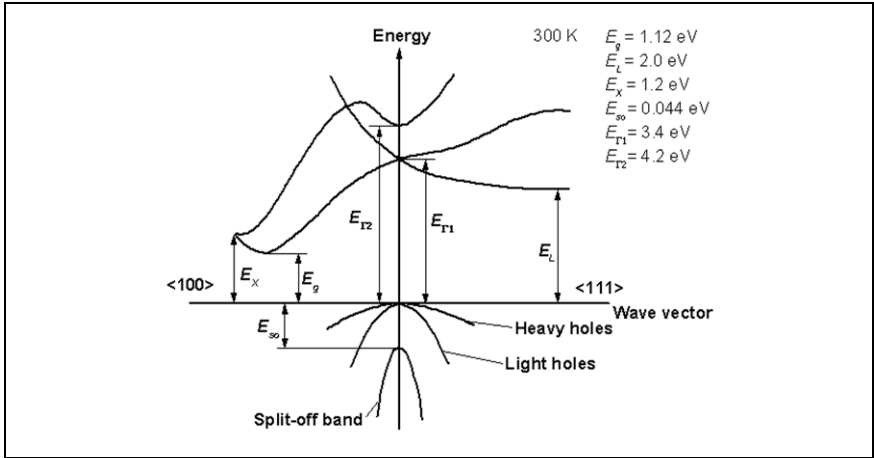


Figure 4: Band structure of single-crystal Silicon (figure taken from [12]). E_g = indirect bandgap; E_L = energy gap between the valence band maximum and the L-valley; E_X = energy gap between the valence band maximum and the X-valley; E_{SO} = energy gap due to spin-orbital splitting; E_{T1} , E_{T2} = local direct bandgaps

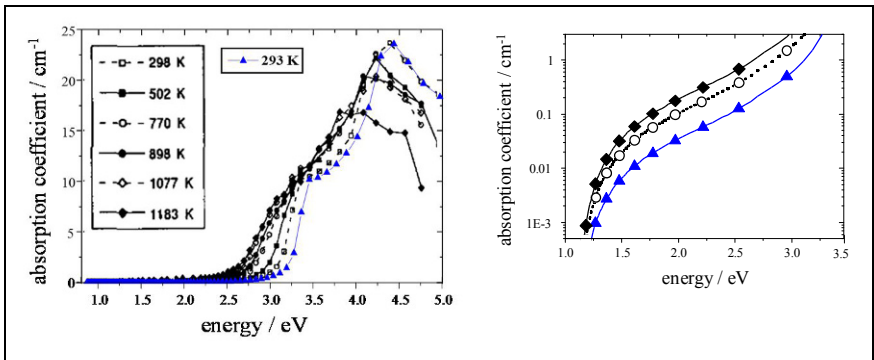


Figure 5: Absorption spectrum for single-crystal Silicon as a function of photon energy and temperature (acc. to [13]). The weak rise in absorptivity around the global indirect bandgap E_g at 1.12 eV at a temperature of 293 K is depicted in the detail on the right hand side (data taken from [14]) along with $\alpha(\lambda, T)$ for two different temperatures according to Equation (3) for comparison (legend of the overall absorption spectrum applies). To prove comparability, the absorptivity $\alpha_0(\lambda)$ at a temperature of 293 K according to Green and Keevers [14] is also shown in the graph on the left hand side in the overall absorption spectrum.

For temperatures T between 298 K and 1183 K and photon energies below E_{T1} Sun et al. found that absorptivity α can be described by

$$\alpha(\lambda, T) = \alpha_0(\lambda) \exp\left(\frac{T}{T_0}\right), \quad (3)$$

whereby $T_0 = 703$ K [13]. The inset in Figure 5 also shows that the drop in absorptivity around the indirect bandgap at a photon energy of 1.12 eV is shifted for elevated temperatures towards decreasing photon energy, i.e. increasing wavelength, according to the bandgap-narrowing with rising temperature. In addition to optical absorption across the bandgap, free carrier absorption or intraband absorption has an impact on the absorption spectrum. The slope in absorptivity at high photon energies, i.e. at short wavelengths, is weaker for elevated temperatures, which may be attributed to a higher reflectivity due to free carrier absorption above the direct bandgap [13]. As will be shown later (cf. subsection 2.3.3), shallow doping leads to large dopant concentrations despite medium implantation doses [15]. Therefore, heavy doping needs to be considered in the following. Figure 6 shows the absorptivity for lightly and heavily doped Silicon [16]. Figure 6 and Figure 7 exhibit the absorption spectrum for increasing dopant (Boron) concentration. The slope of the graphs can be well explained by enhanced free carrier absorption [16]. This results in a conversion from an absorption edge into an absorption minimum.

In the presence of (dopant) impurities zero-phonon interband transitions may be observed. To investigate this effect, the authors subtracted the influence of intraband and free carrier absorption by an electron gas model to deduce the dependence on optical absorption across the bandgap as a function of incident photon energy which is depicted in Figure 7. Zero-phonon transitions should result in a steeper slope of the absorption curve for higher dopant concentrations which is merely the case [16]. Moreover, no significant band-gap shift for different concentrations can be found.

Opposing to the expected bandgap narrowing for heavy doping due to intraband levels, there is a concurrent process known as the Burstein-Moss effect as a consequence of the shift of the Fermi energy level into the valence band for heavy p-type doping. Partial band-filling of the valence band with holes leads to a higher photon energy necessary to raise a bound electron from the valence band into the conduction band although this effect is more pronounced for n-type doping. These opposite effects lead to a so-called band gap renormalisation [16], [17].

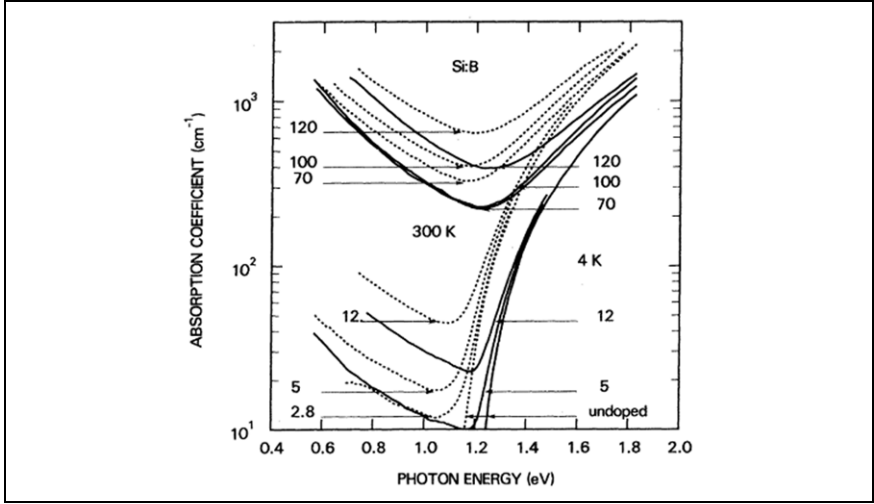


Figure 6: Absorption spectrum for various dopant concentrations (in units of 10^{18} cm^{-3}) measured at temperatures of 4 K and 300 K (figure taken from [16]).

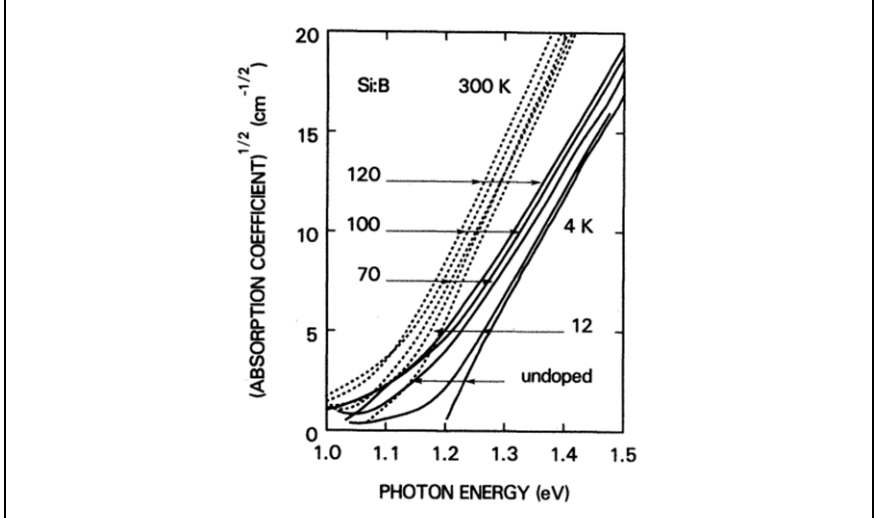


Figure 7: Square root of the absorption coefficient to show optical absorption across the bandgap. Free carrier absorption has been removed by a model based on interacting electron-gas from Figure 6. Concentrations are given in units of 10^{18} cm^{-3} (figure taken from [16]).

Incident photons are primarily absorbed through electron-hole-formation via the bandgap. Excessive photon energy is subsequently released to the lattice by electron-phonon-coupling. The resulting change in thermal energy dQ during a temperature interval dT at constant volume V or constant pressure p is defined as heat capacity

$$C_{V,p} = \left| \frac{dQ}{dT} \right|_{V,p}. \quad (4)$$

There are two results for C_V depending on the model that is applied: For the calculation of the mean thermal energy Q Einstein viewed the atoms of a semiconductor lattice as harmonic oscillators moving independently with the same frequency ν_E at temperature T . Debye, however, considered phonons in a box with a frequency spread $d\nu$. The general description of Q can be expressed by

$Q = \langle n(E) \rangle E$, where

$$\langle n(E) \rangle = \frac{1}{\exp\left(\frac{h\nu}{k_B T}\right) - 1} \quad (5)$$

refers to the mean occupation number according to the Bose-Einstein statistics, E indicates the phonon energy, k_B the Boltzmann constant, h indicated Planck's constant and ν represents the frequency.

Following Einstein's theory, where the lattice atoms are treated as independently moving harmonic oscillators with equal frequency ν_E , the heat capacity

$$C_V = 3 N_A h \nu_E \frac{1}{(\exp\left(\frac{h\nu_E}{k_B T}\right) - 1)^2} \exp\left(\frac{h\nu_E}{k_B T}\right) \frac{h\nu_E}{k_B T^2}. \quad (6)$$

is obtained using Equation (5) to perform Equation (4), whereby N_A represents the Avogadro constant. Debye's approach considers phonons as a gas in a box with a volume V and with a frequency range $d\nu$ to give a thermal energy of

$$Q = 3 \frac{V^3 \nu^2}{2\pi^2 c_s^3} \int_0^{\nu_D} E d\nu \quad (7)$$

whereby ν_D denotes the Debye frequency and c_s the phonon propagation speed in the solid.

Thus, for Debye's theory C_V is expressed by

$$C_V = 9Nk_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D} \frac{\frac{h\nu}{k_B T} \exp\left(\frac{h\nu}{k_B T}\right)}{\left(\exp\left(\frac{h\nu}{k_B T}\right) - 1\right)^2} d\nu \quad (8)$$

In the high temperature limit both results approach $3N_A k_B (= 24.9 \text{ Jmol}^{-1} \text{K}^{-1})$ at a temperature which is known as the Debye temperature $\theta_D = \frac{\hbar\omega_D}{k_B}$. This upper limit agrees with the value due to the Dulong-Petit law which is derived from the equipartition theorem according to which each mode in a monoatomic solid carries the energy $Q = 3N_A k_B T$. Equation (4) thus yields a heat capacity of $3N_A k_B$ as found above. For Silicon this limit corresponds to a heat capacity of $0.89 \text{ Jg}^{-1} \text{K}^{-1}$ at a temperature of 636 K [18].

Knowing C_V , the heat capacity at constant pressure C_p can be obtained from the thermodynamics for cubic solids. For a solid having a linear expansions coefficient α , an isothermal compressibility κ_T and a volume V , C_V and C_p differ at temperature T by

$$C_p - C_V = \alpha^2 V T \frac{1}{\kappa_T}. \quad (9)$$

The difference in absolute values is negligible. However, in contrast to C_V , C_p continues to increase above the Debye temperature, which is mainly due to the fact, that the coefficient of linear expansion for Silicon as the compressibility of solids can be neglected.

Experimental results for C_V and C_p are shown in Figure 8. The dotted line indicates estimates due to the Dulong-Petit law. At low temperatures C_p and C_V are almost indistinguishable. At elevated temperatures, however, C_p violates this law and increases above the Debye temperature.

The distribution of temperature T in space x and time t is described by the differential heat equation

$$\frac{\partial}{\partial t} T(x, t) - \frac{\lambda}{\rho c} \frac{\partial^2}{\partial x^2} T(x, t) = 0 \quad (10)$$

for the one-dimensional case, whereby λ_c specifies the thermal conductivity, ρ the material density and c the specific heat capacity of the material. The specific heat capacity of Silicon has already been looked at. Figure 9 shows experimental data for the thermal conductivity of single-crystal Silicon at temperatures between 2 K and 2000 K [20]. The contributions to the thermal conductivity of Silicon can be distinguished into photon (= radiative contri-

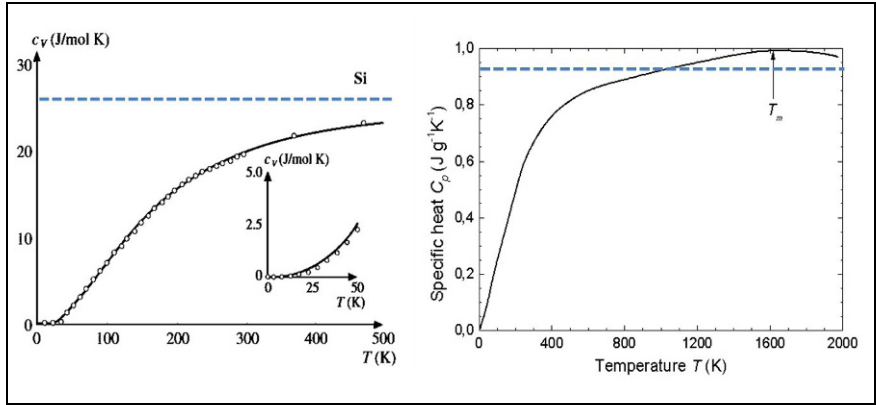


Figure 8: Experimental data for the heat capacity at constant volume (left, taken from [18]) and at constant pressure (right, taken from [19]) for single-crystal Silicon in comparison to the result predicted by the Dulong-Petit law (dotted line).

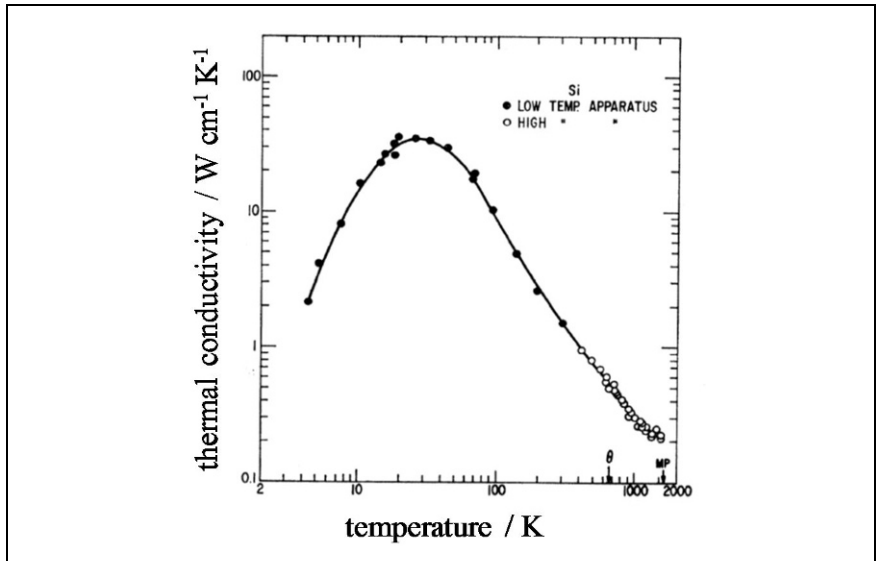


Figure 9: Thermal conductivity of Silicon at temperatures between 2 K and 2000 K. The results have been produced with two apparatus for the low (solid circles) and high temperature regime (open circles), (figure taken from [20]).

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Annealing

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