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EFFECT OF SURFACE AND GRAIN BOUNDARY ON LATTICE THERMAL CONDUCTIVITY OF POLYCRYSTALLINE SILICON LAYERS

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ABSTRACT

Effect of grain boundary scattering on the lattice thermal conductivity of polycrystalline silicon layer has been calculated by describing a linear relation of the grain size in a non-homogeneous grain structure of polysilicon. The effects of surface and size, on the thermal conductivity of polycrystalline material, has been studied by Mayadas and Shatzkes with the solutions of the Boltzmann equation within relaxation time approximation. We have combined the two approaches using Mattheissen's rule to analyze dependence of temperature on the thermal conductivity of doped and undoped polysilicon layers of 1μm thickness between 20-300K. The calculations show a deviation in the thermal conductivity curves at low temperatures, which can be due to the average grain size that is being considered for the analysis. The deviation between theory and experiment may also be due to the fact that Mayadas and Shatzkes theory is the extension of the Fuchs-Sondheimer theory, which may not be suitable for such low dimensions, and more work is required to modify FS theory for film of nanosizes.

INTRODUCTION

Polycrystalline silicon layers are widely used for microelectronic devices and micro-electromechanical systems of micrometer thickness. The thermal conductivity of the polycrystalline layers is drastically reduced as compared to single crystal layers of the substance. The presence of the grains in the polycrystalline layers strongly governs the reduction of the thermal conductivity. The effects of size and surface of the layers is also a factor to cause a reduction in the thermal conductivity.

MODEL FOR POLYCRYSTALLINE LAYER

The phonon scattering in a polycrystalline layer[1] is strongly influenced by the local varying grain size and the layer boundaries. The phonon transport can be obtained by the integration along the layer with a non-homogeneous grain structure and approximated as:

$$\tau_g^{-1} = \frac{v}{d_g}\frac{1-p(\omega)}{1+p(\omega)} \qquad (1)$$

where, v is the phonon group velocity and d_g is the average grain size. The other parameters, which influence the grain boundary scattering, are the surface roughness (η) and the density of related defects surrounding the grain. These effects can be accounted by the specular transmission[2, 3] at the grain boundaries, which effectively increase the grain size, and is given by

$$p(\omega) = \exp\left[-\pi\left(\frac{2\eta\omega}{v}\right)^2\right] \qquad (2)$$

The grain size of the non-homogeneous structure linearly increases from the bottom of the film surface to the top which can be summarized as:

$$d_g(z) = \left[d_{\max} - d_{\min}\right]\frac{z}{d} + d_{\min} \qquad (3)$$

where d_{max}, d_{min} are the maximum and minimum grain sizes respectively while d is the film thickness. We however assume the average grain size as adjustable parameter.

The phonon flux density can be calculated by the simple relation:

$$Q_q = -K(T)\frac{dT}{dz} = \frac{1}{(2\pi)^3}\frac{1}{d}\int_0^d N_q^1 \mathrm{h}\omega_q v_z d^3q dy \qquad (4)$$

which gives the thermal conductivity relation as:

$$\frac{K(T)}{K_0(T)} = \left[1 - \frac{6}{\pi\delta_0}(1-p)\times \int_0^{\pi/2} d\phi \int_1^{\infty} dt \frac{\cos^2\phi}{H^2(t,\phi)}\left(\frac{1}{t^3} - \frac{1}{t^5}\right)\frac{1-\exp\left(-t\delta_0 H(t,\phi)\right)}{1-p\exp\left(-t\delta_0 H(t,\phi)\right)}\right] \qquad (5)$$

where, $\delta_0 = d/l_0$ and $H(t,\phi) = 1 + (\alpha/\cos\phi\sin\theta)$. Here l_0 is the mean free path due to background scattering, $K_0(T)$ [9, 10] is the thermal conductivity of the single crystal layer in the absence of the grains.

The elastic scattering processes for the electron-phonon interaction yields the relaxation time as:

$$\tau_{ep}^{-1} = E_{ep}^{el}\omega_q^4 \qquad (6)$$

where, $E_{ep}^{el} = \frac{(0.33\Xi)^4}{10\pi\rho^2 v^2} 3 w_{ave} \chi^2\left(\frac{\omega}{v_i}\right)\times \left\{\left[v_L^{-5}\chi^2\left(\frac{\omega}{v_L}\right)\right] + \left[v_L^{-5}\chi^2\left(\frac{\omega}{v_{TO}}\right)\right]\right\}\frac{2\Delta^2}{\left(\Delta^2 - \mathrm{h}^2\omega^2\right)} 2n_o$

Here, Ξ is the shear deformation potential, $w_{ave} = 0.66$ is the average angular weight function, $\Delta = 13\,meV$ is the energy difference between the singlet and doublet states, ρ is the mass density of the crystal. n_o represents the number of electrons in the non-metallic state. The parameter $\chi(q) = \left\{1 + 0.25\left(a_B\right)^2 q^2\right\}^{-2}$, where, q is the phonon wave vector and a_B is 66A^o is the effective Bohr radius. E_{ep}^{el} depends on the deformation potential[4] and shape factor as derived by Griffin and Carruthers[5]. The thermal conductivity of the doped single crystal silicon layer further reduces below the thermal conductivity maximum as shown in Fig. 4. The dopants, therefore, acts as the impurity centers modifying the mass-difference scattering parameter, which affects the reduction of the thermal conductivity below its maximum. The calculations show a reasonably good agreement between theory and experiment as plotted in Fig.1.

The thermal conductivity of the polysilicon layer can therefore be analyzed with reasonable agreement by using average grain size in eqns. (1 and 5), i.e., by combining Uma et.al. model with the modified Fuchs[6]-Sondheimer[7] relation.

The deviation at high temperatures can be due to the fact that the umklapp three-phonon scattering processes require the modifications due to thickness of the film as observed previously during the study of the phonon confinement in the thin films and wires.

The reduction of the thermal conductivity of the polycrystalline silicon layer as compared to single crystal silicon layer (Fig.2) has been analyzed by considering the present so called phenomenological model which assumes the average grain size in eqn. (1) for the grain boundary scattering and the relaxation times are modified by the shape factor obtained by Mayadas and Shatzkes[8]. The analysis of the thermal conductivity of polysilicon crystal is done by considering the average size of the grains with shape factor. It can be due to the averaging of the grain size and the surface roughness. Uma[9] et. al. have suggested the method to account the effect of the varied grain size but the simultaneous consideration of grain size and shape factor creates difficulties in computation, which can be simplified only by decoupling the two effects. This decoupling may be achieved only by taking average grain size.

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TABLES

TABLE I

Parameter (unit)	Value used in the analysis
v (cm/sec)	6.64×10^{5}
A (sec ^{3})(bulk)	2.0×10^{-45}
A (sec ^{3}) (undoped single crystal layer)	1.0×10^{-45}
A (sec ^{3}) (doped single crystal layer without electron-phonon interaction)	3.0×10^{-45}
A (sec ^{3}) (doped single crystal layer with electron-phonon interaction)	1.1×10^{-45}
A (sec ^{3}) (undoped polycrystalline layer)	4.0×10^{-43}
A (sec ^{3}) (doped polycrystalline layer without electron-phonon interaction)	2.0×10^{-44}
A (sec ^{3}) (doped polycrystalline layer with electron-phonon interaction)	6.0×10^{-44}
B_L (sec K^{-3})	0.70×10^{-24}
B_{TO} (K^{-3})	9.30×10^{-13}
η (nm) (undoped single crystal layer)	0.276
η (nm) (doped single crystal layer without electron-phonon interaction)	0.970
η (nm) (doped single crystal layer with electron-phonon interaction)	1.00
η (nm) (undoped polycrystalline layer)	0.50
η (nm) (doped polycrystalline layer without electron-phonon interaction)	0.50
η (nm) (doped polycrystalline layer with electron-phonon interaction)	0.50
L (cm)	0.44
d (μm)	1.00
R	0.20
B_{TU} (sec)	5.50×10^{-18}

FIGURES

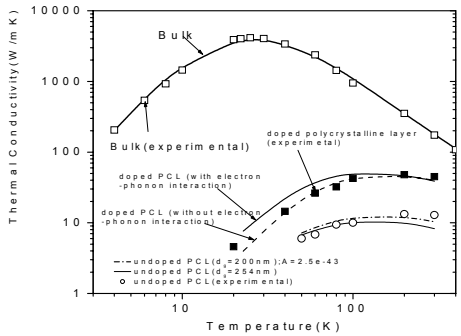

Fig.1. Temperature vs. thermal conductivity of bulk silicon compared with the silicon polycrystalline layer (PSL) (doped and undoped)

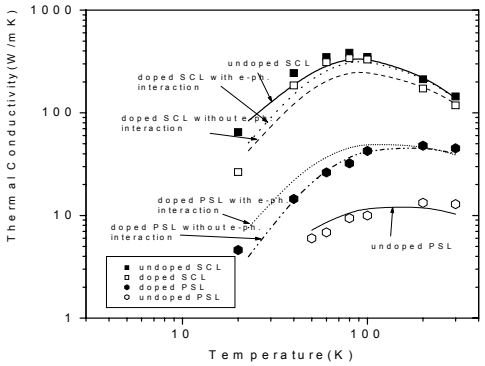

Fig.2. Temperature vs. thermal conductivity of silicon single crystal layer (doped and undoped) compared with polycrystalline silicon layer (doped and undoped)