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Ultrasonic attenuation in pure and doped *n*-type silicon

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The attenuation due to phonon viscosity and thermoelastic phenomena of longitudinal ultrasonic waves propagating along ⟨100⟩ and ⟨110⟩ directions and shear waves polarized along ⟨100⟩ and ⟨110⟩ directions, has been evaluated for pure and doped *n*-type silicon at 298 °K using second- and third-order elastic moduli through Grüneisen mode $\langle \gamma \rangle$, average square Grüneisen constant $\langle \gamma^2 \rangle$, and nonlinearity constant D. The present theoretical results of pure silicon for longitudinal and shear waves along ⟨100⟩ direction are in good agreement with the previous experimental results. The phonon viscosity in terms of dislocation-drag coefficient along ⟨100⟩ and ⟨110⟩ directions is also discussed.

INTRODUCTION

Out of the three thermal causes[1] of acoustic attenuation in solids, only the phenomenon of phonon-viscosity loss, i.e., Akhieser loss,[2] where the energy conversion takes place due to thermal conduction between the phonons at different temperatures and thermoelastic phenomenon owing to the thermal conduction between the compressed and rarefied parts of acoustic waves, suffice to account for most of the attenuation suffered by waves in insulating[3] and conducting[4] crystals. For a thorough study of smooth variation of thermoelastic attenuation from insulating to conducting crystals, we have recently studied the ultrasonic attenuation in pure and doped germanium[5] and its properties are found to be in between metal[4] (conducting) and insulating[3] (dielectric) crystals. In the present investigation we have studied theoretically the acoustic-wave attenuation due to Akhieser loss and thermoelastic loss along with the phonon viscosity in terms of the dislocation-drag coefficients (screw and edge) for pure and doped (with *n*-type impurity) silicon at 298 °K.

Second- and third-order elastic moduli

Keyes[6] has predicted that doping in Si would produce a measurable change in their elastic constants. The two sets of data for a doping concentration of 2×10^{19} atoms of phosphorus per unit volume of Si by Hall[7] are given in Table I.

THEORY

The attenuation due to phonon-viscosity mechanism is obtained from

$$\alpha_1 = \frac{E_0 \omega^2 (D_L/3)\, \tau_L}{2\rho V_L^3}, \qquad (1)$$

where the condition $\omega \tau_{\text{th}} \ll 1$, viz., the time period of propagating wave $1/\omega$ is much greater than the thermal relaxation time τ_{th} has been assumed. Here E_0 is the thermal energy density, ω is the angular frequency, ρ is the density, V_L is the velocity of the longitudinal ultrasonic wave, and D_L is acoustic coupling constant.

A similar relation holds for shear wave. The thermal relaxation time for longitudinal wave (τ_L) is twice the value of shear wave (τ_S) as

$$\tau_L = 2\tau_S = 2\tau_{\text{th}} = 2.\,3K/C_V \langle V \rangle^2 , \qquad (2)$$

where K is the thermal conductivity, C_V is the specific heat per unit volume, and $\langle V \rangle$ is the Debye average velocity. The acoustic coupling constant D in Eq. (1) is obtained from the second- and third-order elastic moduli using the formulas of γ_i^j and

$$D = 9 \langle (\gamma_i^j)^2 \rangle - 3 \langle \gamma_i^j \rangle^2 \, (C_V T/E_0) , \qquad (3)$$

where γ_i^j is the Grüneisen number corresponding to a particular direction of propagation and polarization. The thermoelastic attenuation is obtained from

$$\alpha_1 = \omega^2 \langle \gamma_i^j \rangle^2 \, KT/2\rho V_L^5 .$$

This type of attenuation takes place only in longitudinal wave, because in shear wave propagation, the volume remains unaltered and there is no heating effect which makes this contribution nil. The mathematical formulation of phonon viscosity associated with the two types of waves and dislocation drag coefficients are given elsewhere.[4]

TABLE I. Second- and third-order elastic moduli of pure and doped *n*-type silicon in units of 10^{12} dyn/cm^2 at 298 °K.

	Elastic constant	Pure Si	Doped Si
1	C_{11}	1.6564	1.6394
2	C_{12}	0.6394	0.6477
3	C_{44}	0.7951	0.7919
4	C_{111}	−7.95	−6.58
5	C_{112}	−4.45	−5.11
6	C_{123}	−0.75	+0.60
7	C_{144}	+0.15	+0.65
8	C_{166}	−3.10	−3.36
9	C_{456}	−0.86	−0.86

TABLE II. Primary physical constants for pure and doped Si.

State of Si	V_L (m/sec)	V_S (m/sec)	$\langle V\rangle$ (m/sec)	C_V 10^7 (erg cm^{-3} °K^{-1})	E_0 10^7 (erg cm^{-3})	τ_{th} (10^{-11} sec)
Pure	8431	5843	6354	1.654	2.523	0.7628
Doped	8387	5830	6336	1.658	2.537	0.5853

RESULTS AND DISCUSSIONS

Table II lists the values of primary physical constants calculated for pure and doped silicon, where the values of V_L, longitudinal wave velocity and V_S, shear acoustic wave velocity have been evaluated with the help of the second-order elastic constants C_{11}, C_{44}; density values and weighted average of their cubes leads to Debye average velocity. The values of specific heat per unit volume, C_V, as a function of (Θ/T) have been taken from the literature.[8] Thermal energy density E_0 and thermal relaxation time τ_{th} have been evaluated therefrom [by Eq. (2)] with the help of thermal conductivity values of pure and doped silicon[9] for a doping concentration of 2×10^{19} atoms of phosphorus per unit volume.

The cubic nature of silicon lattice is unaffected by doping[9] thus Mason's theoretical formulas[10,11] for various phonon branches are unaffected; γ_i^j values have been evaluated with Mason's formulas with the help of second- and third-order elastic moduli. For the longitudinal as well as shear acoustic waves propagating along ⟨100⟩ and ⟨110⟩ (⟨1$\bar{1}$0⟩ for shear wave) directions, a weighted average of these mode gammas over 39 pure modes have been taken. The values thus obtained for average Grüneisen constant $\langle\gamma\rangle$, average square Grüneisen constant $\langle\gamma^2\rangle$ and acoustic coupling constant D, by Eq. (3) are presented in Table III. $\langle\gamma\rangle$ values are zero for shear wave, and thus thermoelastic attenuation is zero in this case. For longitudinal wave propagating in pure silicon along ⟨100⟩ direction, the present value of $D=5.3085$ lies between the results of McSkimin *et al.*[12] ($D=5.25$) and Drabble *et al.*[13] ($D=5.45$). Also for the shear wave along ⟨100⟩ direction the present value of $D=0.7785$ is very close to earlier work of McSkimin *et al.*[12] ($D=1.0$), and Drabble *et al.*[13] ($D=0.94$). As a result of doping there is a general increase in all these parameters.

The total attenuation consists of two parts: Akhieser loss and thermoelastic attenuation. The attenuation due to Akhieser loss is found to be dominating as compared to the thermoelastic loss (see Table IV) which shows that the major part of the ultrasonic energy loss is used in achieving the equilibrium among various phonon branches and directions at different temperatures. The latter's contribution is only 2.4% of the former as compared to 3.6% for Ge, 4% for CaF_2 (Ref. 14) (dielectric crystal), and 50% for silver (metal crystal). This shows that the properties of the semiconductor lies between metal and insulators.

Considering the contribution from the above two thermal causes, the total ultrasonic attenuation for longitudinal and shear waves propagating along ⟨100⟩ direction are shown in Figs. 1 and 2, respectively.

The experimental results in pure Si of Mason and Bateman[10] for longitudinal waves (2.18 dB/cm at 480 MHz and 0.77 dB/cm at 286 MHz) and shear wave (0.72 dB/cm at 495 MHz) along ⟨100⟩ directions are in good agreement with the present theoretical results (1.975, 0.702, and 0.892 dB/cm) for longitudinal and shear waves, respectively. For pure silicon the experimental points lie almost on the theoretical curves (Figs. 1 and 2).

The theoretical ultrasonic attenuation for longitudinal and shear waves in Si increases due to doping by 10 and 18%, respectively, as compared to 27 and 73% for germanium.[5] No experimental result is available for *n*-type doping though it exists for *p*-type doping.[15,16] The nice agreement achieved for pure silicon is a sufficient basis for the pre-

TABLE III. Grüneisen number and nonlinearity constant along ⟨100⟩ and ⟨110⟩ directions for pure and doped Si.

Direction	State of Si	$\langle\gamma\rangle$ Long	$\langle\gamma\rangle$ Shear	$\langle\gamma^2\rangle$ Long	$\langle\gamma^2\rangle$ Shear	D Long	D Shear
⟨100⟩	Pure	0.4778	00	0.7385	0.0865	5.3085	0.7785
	Doped	0.5981	00	1.0540	0.1298	7.3970	1.1682
⟨110⟩[a]	Pure	0.4784	00	0.5399	0.6566	3.5181	5.9094
	Doped	0.7280	00	0.7442	1.2540	3.6028	11.2860

[a] For shear waves, $\langle\gamma^2\rangle$ and D are along ⟨1$\bar{1}$0⟩.

TABLE IV. Attenuation of longitudinal and shear acoustic wave and drag coefficient of screw and edge dislocation along ⟨100⟩ and ⟨110⟩ directions. Akh represents Akhieser and Therm represents thermoelastic.

Direction	State of Si	$(\alpha/f^2)_{\text{Akh}}$ (10^{-17}dB sec^2 cm^{-1}) Long	Shear	$(\alpha/f^2)_{\text{Therm}}$ (10^{-18}dB sec^2/cm) Long	B_{screw} (10^{-2} P) Long	Shear	B_{edge} (10^{-2} P) Long	Shear
⟨100⟩	Pure	0.8371	0.3641	0.2018	0.4838	0.0350	0.6228	0.0743
	Doped	0.9141	0.4298	0.2456	0.5200	0.0412	0.6707	0.0821
⟨110⟩[a]	Pure	0.5547	2.7050	0.2023	0.3206	0.2601		
	Doped	0.4451	4.1510	0.3638	0.2532	0.3966		

[a] For shear waves polarization are along ⟨1$\bar{1}$0⟩ direction.

diction of the results for doped silicon. A similar set of results has been tabulated in Table IV for longitudinal wave along ⟨110⟩ direction and shear wave polarized along ⟨1$\bar{1}$0⟩ direction. But here, as before (as for ⟨100⟩) the attenuation of shear wave increases on doping in contrast to Ge[5] where it decreases.

Dislocation-drag coefficient have been evaluated using equations given in an earlier paper.[4] Doping, which tends to convert an insulator into a semiconductor is accompanied by an increase in the acoustic coupling constant D. This increase of D, increases the phonon viscosity which creates a greater resistance against the motion of moving dislocation. The results obtained are shown in Table IV.

CONCLUSIONS

From Tables III and IV it is found that as a result of doping by phosphorus atom (n-type) a general increase ranging from 10 to 54% (90% increase in D value for shear wave polarized along ⟨1$\bar{1}$0⟩ in different propagation parameters is observed similar to p-Si,[15] except for velocities V_L and V_S, Akhieser loss for longitudinal wave along ⟨110⟩ and B_{screw} (screw-dislocation-drag coefficient) for lon-

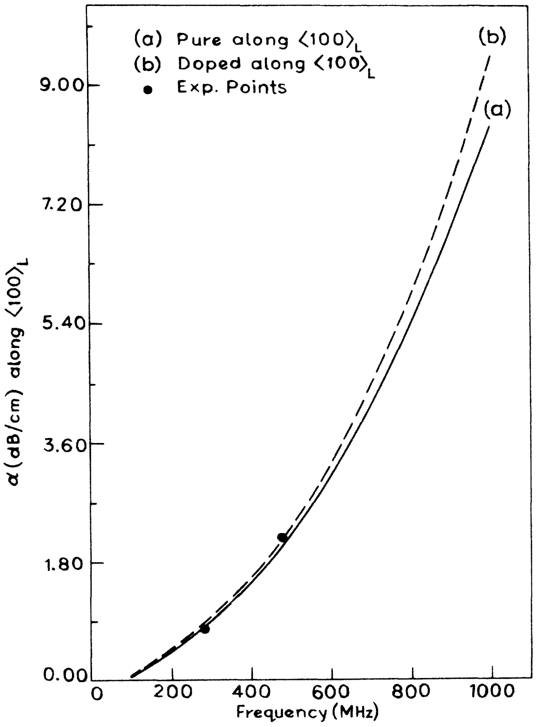

FIG. 1. Variation of attenuation α (dB/cm) with frequency for longitudinal wave in ⟨100⟩ direction. The experimental points of Mason and Bateman (see Ref. 10) are shown.

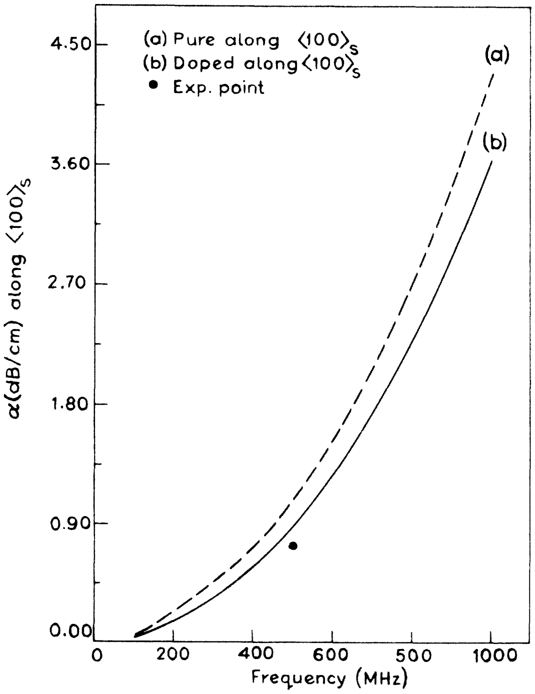

FIG. 2. Variation of attenuation α (dB/cm) with frequency for shear wave polarized along ⟨100⟩ direction. The experimental point of Mason and Bateman (see Ref. 10) is shown.

gitudinal wave along ⟨110⟩ which decreases on doping due to approximately same value of acoustic coupling constant D (3.5181 for pure and 3.6028 for doped) and different thermal relaxation time (0.7628 $\times 10^{-11}$ sec for pure and 0.5853$\times 10^{-11}$ sec for doped). Here for ⟨100⟩ direction, the thermoelastic attenuation which is directly being governed by thermal conductivity is affected to a greater extent than the Akhieser attenuation and shear wave parameters (α_{Akh}) B_{screw}, and B_{edge} show a greater response than their longitudinal counterpart similar to Ge. This nonabrupt rise in attenuation is due to a small doping concentration.

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