# Nonlinear coupling of surface and quasitransverse bulk modes in cubic crystals[a]

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In crystals the speed of the surface acoustic wave mode may approach that of the lowest-speed quasitransverse bulk mode in some directions of propagation. Under these circumstances, it is possible for energy to be transferred from the surface mode to the bulk mode by nonlinear coupling. In the present paper we investigate the possibilities for mode coupling in the (001), (110), and (111) planes of cubic crystals. A condition is given for determining the range of propagation directions with significant coupling, and numerical results are provided for eight different crystals with a range of anisotropy ratios. It is shown that even for significant excitation amplitudes the coupling is negligible for most propagation directions in the aforementioned surface cuts. © *2003 Acoustical Society of America.* [DOI: 10.1121/1.1566974]

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## I. INTRODUCTION

Anisotropic media have the property that acoustic wave speeds vary as a function of the direction of propagation. In particular, there exist directions where the lowest speed of a quasitransverse bulk wave approaches the speed of the surface acoustic wave (SAW).[1] In these instances, it is possible for nonlinear coupling (and therefore energy exchange) between the surface acoustic wave and quasitransverse bulk wave to occur. Several theoretical models for the nonlinear propagation of SAWs in anisotropic media[2–4] do not account for this coupling, an observation also made previously in the context of nonlinear Scholte waves.[5] To properly use these theories it is important to quantitatively determine their regions of applicability, a topic that does not appear to have been explored.

In this article we describe the condition under which significant coupling may be expected in crystals. Calculations based on the model of Ref. 4 are presented for eight different cubic crystals with a range of anisotropy ratios for propagation in the (001), (110), and (111) surface cuts. The properties of nonlinear SAWs in the materials and surface cuts presented here have been discussed in detail in previous work,[6–8] and measurements of finite-amplitude SAWs in selected directions in the (001) and (111) planes of crystalline silicon have corroborated the waveform evolution predicted by the model.[9,10] The present calculations show that for practical excitation amplitudes, negligible coupling is expected for most propagation directions.

## II. MODE COUPLING CONDITION

Coupling between the surface mode and quasitransverse bulk mode is insignificant when the characteristic nonlinear length scale $\bar{x}$ (e.g., the shock formation distance) is large in relation to the coherence length[11] for the modal interaction. For a SAW of wave number $k$ and speed $c$, this criterion corresponds to

$$\frac{1}{k\bar{x}} \ll \frac{\Delta c}{c_b}, \tag{1}$$

where $\Delta c = |c - c_b|$ and $c_b$ is the speed of the bulk wave. The characteristic nonlinear length scale is

$$\bar{x} = \frac{1}{|\beta|\epsilon k}, \tag{2}$$

where $\beta$ is the coefficient of nonlinearity[6] and $\epsilon$ is the characteristic acoustic strain. Substituting Eq. (2) into Eq. (1) yields

$$\epsilon \ll \frac{\Delta c}{c_b}\frac{1}{|\beta|}. \tag{3}$$

Equation (3) can be used in two ways to develop limits for negligible mode coupling. First, the range of propagation directions with negligible mode coupling can be determined with a given upper bound on the acoustic strain. In SAW experiments with some of the largest amplitudes,[9,10] the maximum applied acoustic strain is $\epsilon = 0.01$. With this condition, the criterion for negligible mode coupling is given by

$$0.1 < (\Delta c/c_b)/|\beta|, \tag{4}$$

providing for a difference of an order of magnitude between both sides of Eq. (3). The actual range may be larger depending on the value of $\epsilon$ for a given data set. Equation (4) is used in Sec. III to evaluate the range of propagation directions

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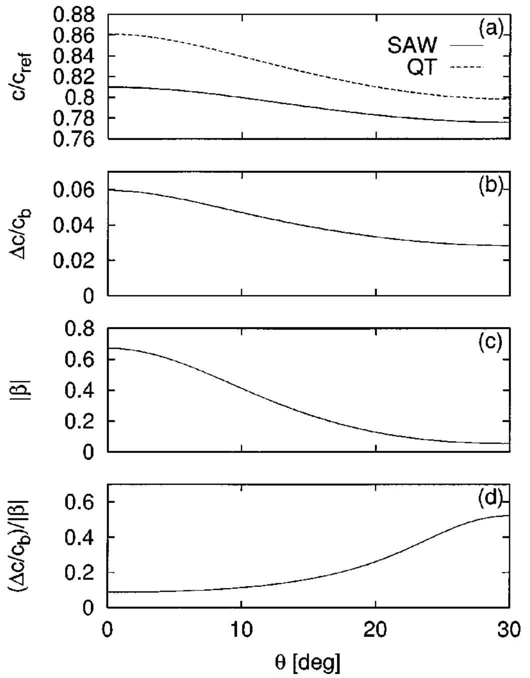


FIG. 1. (a) Scaled SAW and quasitransverse (QT) bulk wave speeds, (b) relative wave speed, (c) nonlinearity coefficient, and (d) ratio of relative wave speed to nonlinearity coefficient as a function of propagation direction for Si in (111) surface cut.

for negligible coupling for a variety of materials and surface cuts. Second, the maximum acoustic strain that ensures negligible mode coupling for all propagation directions is

$$\epsilon_{\max}=\min\left(\frac{\Delta c}{c_b}\frac{0.1}{|\beta|}\right). \tag{5}$$

Values of $\epsilon_{\max}$ for each cut and each material are given in Tables I, II, and III.

## III. RESULTS

### A. Specific case: Si in (111) plane

To illustrate the analysis in detail, calculations are performed for Si in the (111) plane, and the results are summarized in Fig. 1. Figure 1(a) shows the scaled wave speeds $c/c_{\mathrm{ref}}$ of the surface and lowest quasitransverse bulk modes as a function of the angle $\theta$ between the propagation direction and $\langle 11\bar{2}\rangle$, where $c_{\mathrm{ref}}=(c_{44}/\rho)^{1/2}$. Only the angular range $0°\leqslant\theta\leqslant 30°$ is considered because the wave speeds are symmetric about $\theta=30°$ and periodic every 60° in this plane. The speeds approach each other as $\theta\rightarrow 30°$ but do not converge. Figure 1(b) shows $\Delta c/c_b$ as a function of propagation direction. In accordance with Fig. 1(a), the maximum change in relative wave speed occurs at $\theta=0°$ around 5.9% and decreases to around 2.8% as $\theta\rightarrow 30°$. Figure 1(c) shows the magnitude of the nonlinearity coefficient as a function of propagation direction. The magnitude of the nonlinearity coefficient is maximum at $\theta=0°$ and decreases monotonically as $\theta\rightarrow 30°$. (As discussed in Ref. 7, the absolute value of the nonlinearity matrix elements and therefore $|\beta|$ are symmetric about $\theta=30°$ and periodic every 60° in this plane.) Finally,

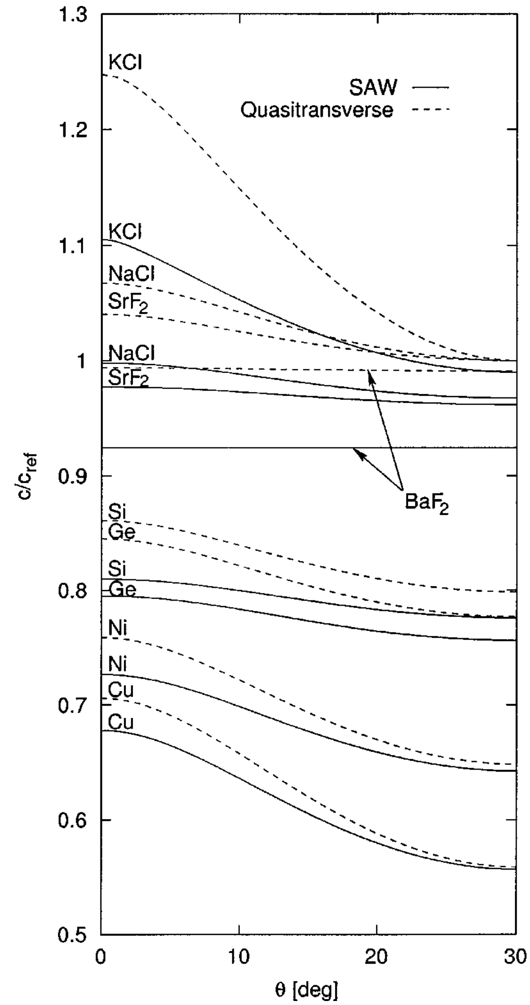


FIG. 2. Scaled SAW (solid) and lowest quasitransverse bulk wave (dashed) mode speeds as a function of propagation direction in the (111) plane.

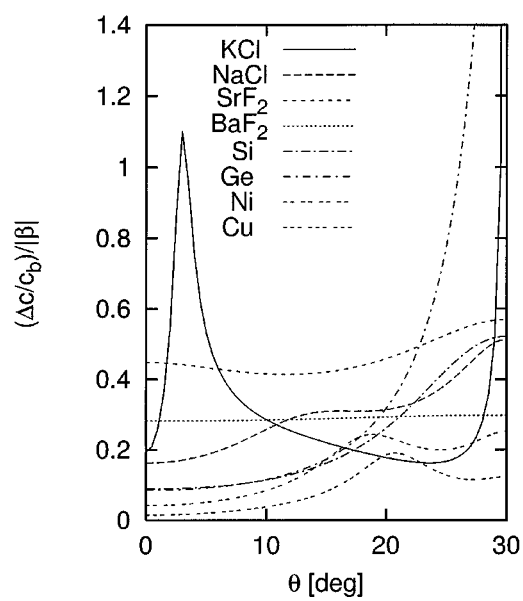


FIG. 3. $(\Delta c/c_b)/|\beta|$ as a function of propagation direction in the (111) plane.

Fig. 1(d) shows $(\Delta c/c_b)/|\beta|$ as a function of propagation direction. While both $\Delta c/c_b$ and $|\beta|$ decrease as $\theta \rightarrow 30°$, their ratio actually increases as $\theta \rightarrow 30°$. Hence, the limitation on the range of negligible mode coupling is due more to the larger nonlinearity coefficient as $\theta \rightarrow 0°$ than to the closeness of the SAW and quasitransverse bulk mode speeds in this region. For this particular case $\epsilon_{max}=0.0088$ by Eq. (5). However, Fig. 1(d) can be used to evaluate the range of propagation directions with negligible coupling for any given value of $\epsilon$ by looking to see where the curve exceeds a horizontal line at that value of the maximum applied acoustic strain.

### B. General study

For many materials, the angular dependence of the SAW speed can be conveniently grouped according to the material's anisotropy ratio[1] $\eta = 2c_{44}/(c_{11}-c_{12})$. The ratio is defined such that $\eta=1$ for isotropic materials. KCl, NaCl, $SrF_2$, $BaF_2$, Si, Ge, Ni, and Cu are selected for study here to illustrate the behavior seen for the range of anisotropy ratios $0.373 \leqslant \eta \leqslant 3.20$. The anisotropy ratio for each individual material is listed in the tables.

#### *1. (111) plane*

Figure 2 shows the scaled surface and lowest quasitransverse mode wave speeds $c/c_{ref}$ as a function of the propagation direction for the (111) plane. As in Fig. 1, $\theta$ is defined as the angle between the propagation direction and $\langle 112 \rangle$. The closest convergence occurs for the materials with $\eta > 1$. Figure 3 shows $(\Delta c/c_b)/|\beta|$ as a function of propagation direction. Table I lists the anisotropy ratios, $\epsilon_{max}$, and the range of directions for negligible mode coupling for values of applied acoustic strain $\epsilon=0.005$ and $\epsilon=0.01$. While the ranges decrease as the anisotropy ratio increases, negligible coupling is expected for most directions in most of the materials. As demonstrated in Sec. III A, the directions without negligible mode coupling tend to occur more where the nonlinearity coefficient is strong rather than where the SAW and quasitransverse bulk modes are nearly equal in speed.

#### *2. (001) plane*

Next, consider propagation in the (001) plane. Figure 4 shows the scaled surface and lowest quasitransverse mode wave speeds $c/c_{ref}$ as a function of propagation distance. In this section $\theta$ is defined as the angle between the propagation direction and $\langle 100 \rangle$. Only the angular range $0° < \theta < 45°$ is

TABLE I. Parameters for mode coupling in the (111) plane.

| Material | $\eta$ | $\epsilon_{max}$ | Negligible mode coupling with $\epsilon=0.005$ | $\epsilon=0.01$ |
|---|---|---|---|---|
| KCl | 0.373 | 0.016 | All directions | All directions |
| NaCl | 0.705 | 0.016 | All directions | All directions |
| $SrF_2$ | 0.803 | 0.041 | All directions | All directions |
| $BaF_2$ | 1.02 | 0.028 | All directions | All directions |
| Si | 1.57 | 0.0088 | All directions | $7° < \theta < 30°$ |
| Ge | 1.66 | 0.0085 | All directions | $7° < \theta < 30°$ |
| Ni | 2.60 | 0.0042 | $5° < \theta < 30°$ | $12° < \theta < 30°$ |
| Cu | 3.20 | 0.0014 | $12° < \theta < 30°$ | $17° < \theta < 30°$ |

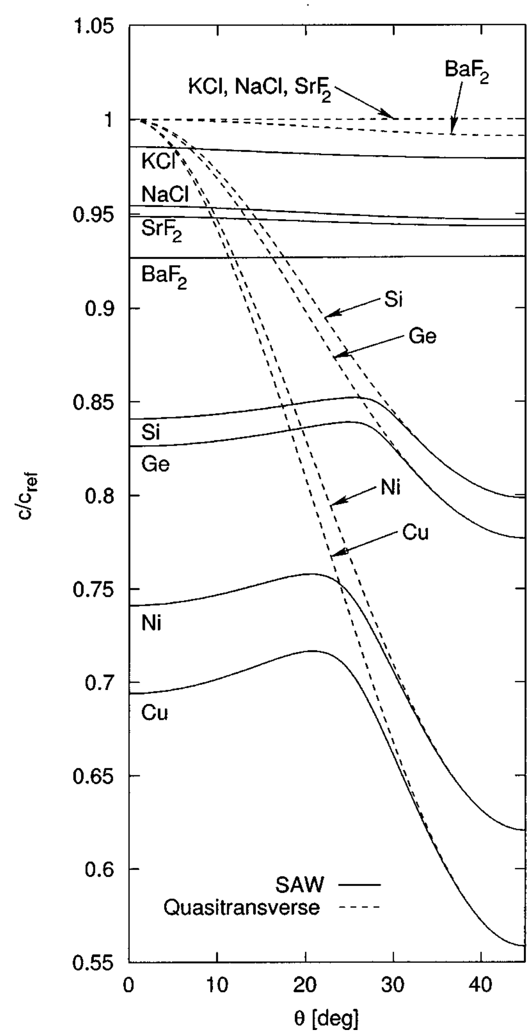


FIG. 4. Scaled SAW and lowest quasitransverse bulk mode speeds as a function of propagation direction in the (001) plane. Note that KCl, NaCl, $SrF_2$ all have $c/c_{ref}=1$.

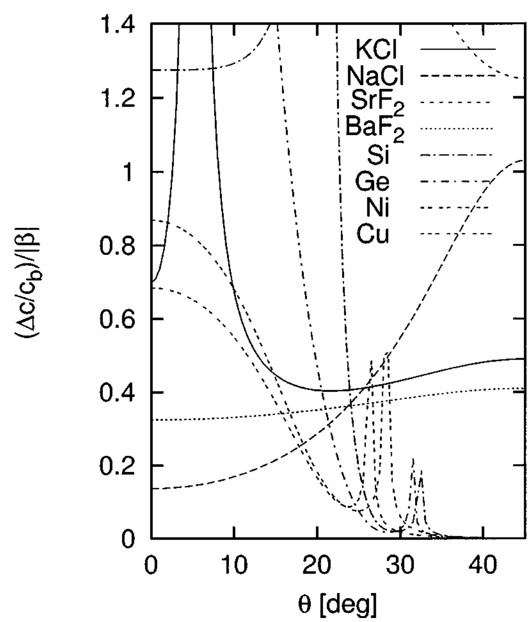


FIG. 5. $(\Delta c/c_b)/|\beta|$ as a function of propagation direction in the (001) plane.

considered because the wave speeds are symmetric about $\theta=45°$ and are periodic every $\theta=90°$. For the materials shown with $\eta>1$, the SAW and lowest quasitransverse bulk modes converge as $\theta\rightarrow 45°$. The pseudosurface wave[1] mode at $\theta=45°$ is not considered in this study.

Figure 5 shows $(\Delta c/c_b)/|\beta|$ as a function of propagation direction. Unlike the (111) plane, $\beta$ is always real-valued in this plane and can be zero.[6] The zeros are the source of the discontinuities in the slope of $|\beta|$ and therefore also in the curves for Si near $\theta=32°$, Ge near $\theta=31°$, Ni near $\theta=26°$ and Cu near $\theta=28°$ in Fig. 5. [In cases where $|\beta|=0$, Eq. (2) does not apply, although an alternative characteristic nonlinear length scale $\overline{x}$ can be constructed[8] so that Eq. (3) is still valid.] Like Table I, Table II lists the acoustic strains and angular ranges with negligible mode coupling. Negligible coupling occurs for all directions for the materials with $\eta<1$. For the materials with $\eta>1$, $|\beta|\rightarrow 0$, but $(\Delta c/c_b)\rightarrow 0$ faster so that the net result is $(\Delta c/c_b)/|\beta|\rightarrow 0$. As a result, negligible mode coupling occurs only in selected ranges, but still over half the possible angular range. Like the (111) plane, the ranges in the (001) plane decrease as the anisotropy ratio $\eta$ increases.

### 3. (110) plane

Finally, consider propagation in the (110) plane. Figure 6 shows the scaled surface and lowest quasitransverse mode wave speeds $c/c_{\mathrm{ref}}$. In this plane, $\theta$ is defined as the angle between the propagation direction and ⟨001⟩. Only the angular range $0°<\theta<90°$ is considered because the wave speeds are symmetric about $\theta=90°$ and are periodic every $\theta=180°$. Note that the discontinuities of the slopes of the lowest quasitransverse mode curves in Fig. 6 occur because the quasitransverse mode of lowest speed changes in these directions from one type to another (e.g., see Figs. 11 and 15 in Farnell[1] for plots of both quasitransverse modes for Ni and KCl). The SAW and lowest quasitransverse bulk mode for KCl and NaCl converge only as $\theta\rightarrow 90°$. While a pseudosurface wave mode is possible at $\theta=90°$ for some materials, it is not considered here.

Figure 7 shows $(\Delta c/c_b)/|\beta|$ as a function of propagation direction. As in the (001) plane, $\beta$ is real-valued and can be zero for certain directions in the materials considered. The zeros or near zeros are the source of the discontinuities in the slope of $(\Delta c/c_b)/|\beta|$ for KCl near $\theta=10°$ and $\theta=70°$, $SrF_2$ near $\theta=11°$ and $\theta=79°$, Si near $\theta=60°$, and Ge near $\theta=65°$. Table III is the analog of Tables I and II for the (110)

TABLE II. Parameters for mode coupling in the (001) plane.

| Material | $\eta$ | $\epsilon_{\max}$ | Negligible mode coupling with $\epsilon=0.005$ | $\epsilon=0.01$ |
|---|---|---|---|---|
| KCl | 0.373 | 0.040 | All directions | All directions |
| NaCl | 0.705 | 0.014 | All directions | All directions |
| $SrF_2$ | 0.803 | 0.12 | All directions | All directions |
| $BaF_2$ | 1.02 | 0.032 | All directions | All directions |
| Si | 1.57 | None | $0°<\theta<27°$ | $0°<\theta<26°$ |
| Ge | 1.66 | None | $0°<\theta<26°$ | $0°<\theta<24°$ |
| Ni | 2.60 | None | $0°<\theta<28°$ | $0°<\theta<22°$ |
| Cu | 3.20 | None | $0°<\theta<30°$ | $0°<\theta<22°$ |

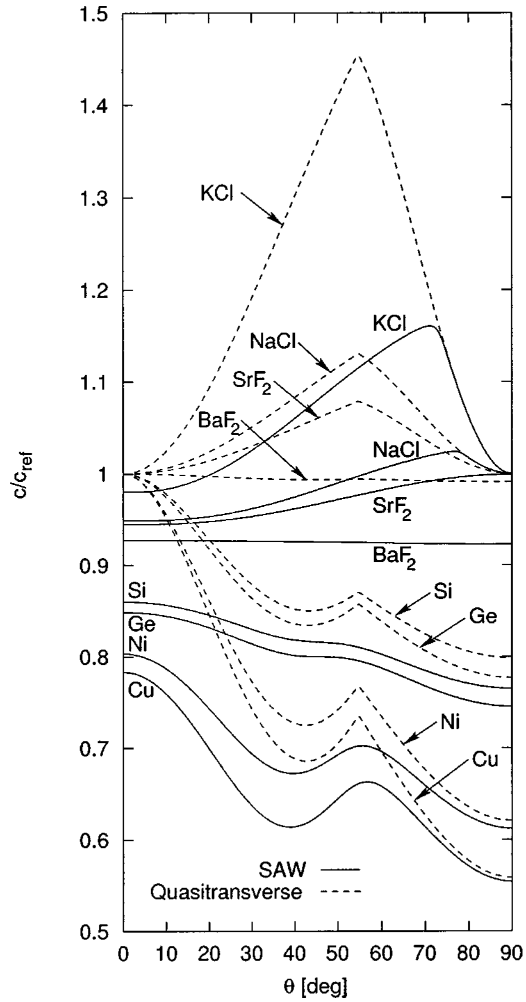


FIG. 6. Scaled SAW and lowest quasitransverse bulk mode speeds as a function of propagation direction in the (110) plane.

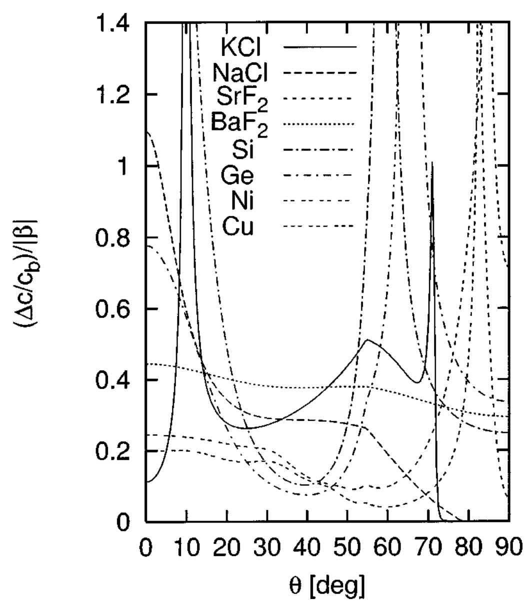


FIG. 7. $(\Delta c/c_b)/|\beta|$ as a function of propagation direction in the (110) plane.

TABLE III. Parameters for mode coupling in the (110) plane.

| Material | $\eta$ | $\epsilon_{max}$ | Negligible mode coupling with $\epsilon=0.005$ | $\epsilon=0.01$ |
|---|---|---|---|---|
| KCl | 0.373 | None | $0°<\theta<72°$ | $0°<\theta<72°$ |
| NaCl | 0.705 | None | $0°<\theta<72°$ | $0°<\theta<67°$ |
| $SrF_2$ | 0.803 | 0.0064 | All directions | $0°<\theta<88°$ |
| $BaF_2$ | 1.02 | 0.029 | All directions | All directions |
| Si | 1.57 | 0.010 | All directions | All directions |
| Ge | 1.66 | 0.0076 | All directions | $\theta<32°;\theta>47°$ |
| Ni | 2.60 | 0.0090 | All directions | $\theta<48°;\theta>61°$ |
| Cu | 3.20 | 0.0040 | $\theta<55°;\theta>65°$ | $\theta<45°;\theta>72°$ |

plane. For KCl and NaCl, $\Delta c/c_b \to 0$ and $|\beta|\to 0$ as $\theta\to 90°$, but the wave speeds converge faster, so that the net result is that the ratio goes to zero. As a result, negligible mode coupling is expected only for propagation directions away from $\theta=90°$, as shown in Table III. For materials with $\eta>1$, negligible coupling is expected for most directions, except for relatively small regions where there is both a strong nonlinearity coefficient and relatively close SAW and quasitransverse wave speeds. As in the previous two planes, the ranges tend to decrease as the anisotropy ratio $\eta$ increases.

## IV. CONCLUSION

The condition for the nonlinear mode coupling between the SAW and lowest quasitransverse bulk mode is defined and examined. Numerical results are presented for the cubic crystals KCl, NaCl, $SrF_2$, $BaF_2$, Si, Ge, Ni, and Cu in the (001), (110), and (111) planes. As an example, a detailed study is provided for Si in the (111) plane. Criteria are developed for (1) determining the range of directions of negligible mode coupling for a given acoustic strain and (2) calculating the maximum acoustic strain for which negligible mode coupling occurs in all directions in a given plane.

In the (111) plane, the magnitude of the nonlinearity coefficient tends to determine the range of directions with negligible mode coupling more strongly than the closeness of the SAW and quasitransverse speeds. In the (001) plane, the nonlinearity coefficient also tends to dominate, except for materials such as Si, Ge, Ni, and Cu, where the SAW and quasitransverse modes converge in speed near ⟨110⟩ ($\theta=45°$). In the (110) plane, regions without negligible mode coupling tend to occur where there is both a relatively strong nonlinearity coefficient and relatively close SAW and quasitransverse wave speeds. Exceptions are KCl and NaCl, where the convergence between the modes in speed near ⟨110⟩ ($\theta=90°$) dominates. The angular ranges of negligible mode coupling for all three planes tend to decrease in size as the anisotropy ratio increases. For typical excitation amplitudes, the results indicate that negligible mode coupling is expected for most propagation directions in the (001), (110), and (111) planes for the materials considered.

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