Unlocking high hole mobility in diamond over a wide temperature range via efficient shear strain

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ABSTRACT

As a wide bandgap semiconductor, diamond holds both excellent electrical and thermal properties, making it highly promising in the electrical industry. However, its hole mobility is relatively low and decreases with increasing temperature, which severely limits further applications. Herein, we proposed that the hole mobility can be efficiently enhanced via slight compressive shear strain along the [100] direction. The shear strain breaks the symmetry of the crystalline structure and lifts the band degeneracy near the valence band edge, resulting in a significant suppression of interband electron-phonon scattering. Moreover, the hole mobility becomes less temperature-dependent due to the decrease of electron scatterings from high-frequency acoustic phonons.

INTRODUCTION

Enhancing carrier mobility is essential for improving the performance and reducing the power consumption of next-generation electronic devices, particularly in high-frequency and high-power applications.[1] Diamond is a rising star semiconductor owing to its ultra-wide bandgap, ultra-high thermal conductivity, and high saturation carrier velocity.[2] However, the hole mobility of diamond is relatively lower compared to its electron mobility and dramatically decreases with increasing temperature.[3] These drawbacks in hole mobility significantly constrain the potential of diamonds in CMOS, high-power LEDs, and detectors.[4]

Strained silicon technology[5] is effective in promoting the hole mobility of silicon, which has been extensively utilized in industry and drives the ongoing progress of Moore's law. Although the strain engineering on the hole mobility of Si, Ge, and Ge-Sn alloy has been extensively studied, research on the diamond, which possesses a similar face-centered cubic (*fcc*) structure, remains relatively scarce. This may be attributed to the extreme hardness and strength of diamond which are widely considered to render strain implementation nearly impossible. Recently, Dang *et al.*[6] realized uniform elastic strain along the [100], [101], and [111] crystal directions by fabricating micron-nanometer scale bridge structures, thereby making it possible for the widespread application of "strained diamond" in electronic devices. It remains unclear whether strain engineering effectively promotes the hole mobility of diamond and shares a similar mechanism with other group IVA *fcc* semiconductors.

RESULTS AND DISCUSSIONS

The crystalline geometry of the relaxed diamond is *fcc* (space group $Fd\overline{3}m$, no. 227) and its first Brillouin zone (BZ) is a truncated octahedron. The SOC removes the triple degeneracy at the VBM, resulting in the double degeneracy of the heavy-hole (*hh*) and light-hole (*lh*) bands, while the split-off hole (*sh*) band lies 13.4 meV lower in energy, as shown in the insets of Fig. 1(a). In contrast, the crystal symmetry is broken with the slight shear strain applied to the *fcc* diamond. The space group is changed to $I4_1/amd$ (no. 141). As a result, the double degeneracy of the *hh* and *lh* bands is lifted under a 2% shear strain along the [100] directions, arousing a large energy splitting of $\sim$ 0.3 eV (highlighted by light green ribbons in Fig. 1(b).)

Fig. 1(c) shows the phonon-limiting hole drift mobility and Hall mobility of the relaxed diamond. The room-temperature hole mobility of the relaxed diamond is 2820 $\mathrm{cm}^2/(\mathrm{Vs})$. There is a dramatic enhancement in hole mobility when shear strain is applied, as shown in Fig. 1(d). Specifically, the in-plane mobility is increased to 14148 $\mathrm{cm}^2/(\mathrm{Vs})$ under 2% compressive (-2%) shear strain along the [100] direction. Correspondingly, the out-of-plane mobility reaches 8252 $\mathrm{cm}^2/(\mathrm{Vs})$ for the -2% shear strain case. As the shear strain increases to 8%, the enhancement in hole mobility gradually approaches saturation. The in-plane hole mobility reaches 24190 $\mathrm{cm}^2/(\mathrm{Vs})$, which is one order of magnitude larger than that of relaxed diamond and is the highest recorded value in bulk semiconductors. The hole mobility typically decreases exponentially with temperature ($\mu \sim T^{-n}$) since phonons are significantly activated, which degrades the performance of electronic devices. For the relaxed case, the value of exponent *n* in the temperature dependence is -2.01. We show that hole mobility becomes less temperature-dependent for diamonds with shear strains. The exponent *n* values of in-plane hole mobility are located in the range of -1.52 to -1.61.

To understand the increase in the hole mobility induced by shear strains, we further project the interband electron-phonon scattering rates onto the band structure for diamonds without/with strain, as shown in Figs. 1(e) and 1(f). There is a significant reduction in the interband electron-phonon scattering rates for the shear-strained diamond, attributed to the substantial energy splitting in the valence bands. This energy splitting prohibits energy conservation and diminishes the available electron-phonon scattering channels. Moreover, intraband electron-phonon scattering processes are primarily mediated by low-frequency acoustic phonons, while the interband scattering processes are mainly assisted by high-frequency acoustic phonons. The relative increase in the number of low-frequency acoustic phonons with temperature is not as significant as that of high-frequency acoustic phonons. Therefore, the hole mobility for strained diamonds becomes less temperature-dependent.

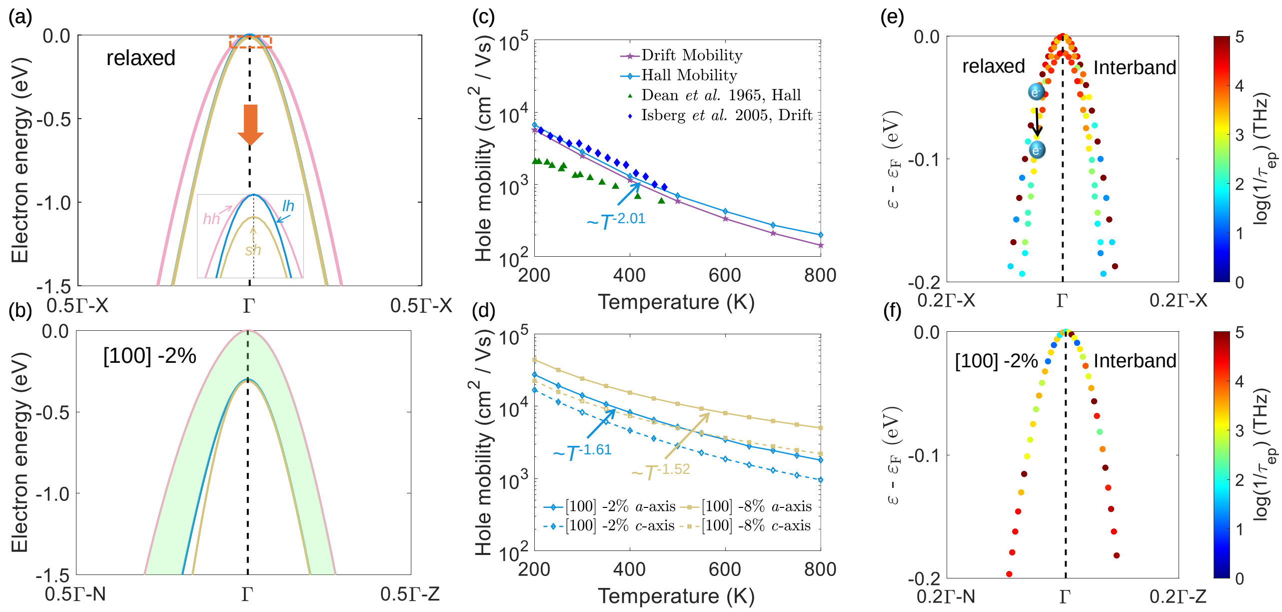

Fig. 1. Valence bands of (a) relaxed structure, (b) the structure with -2% shear strain along the [100] direction. (c) Drift mobility and Hall mobility as a function of temperature for relaxed diamond. The scatters are experimental data reported by Dean *et al.*[7] (triangle) and Isberg *et al.*[8] (diamond). (d) In-plane (*a*-axis) and out-of-plane (*c*-axis) Hall mobilities for shear strains along the [100] directions. Projection of interband electron-phonon scattering rates onto the band structure for (e) relaxed and (f) -2% shear-strained diamond.

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