Theoretical Prediction of Enhanced Thermopower in n-Doped Si/Ge Superlattices Using Effective Mass Approximation

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We analyze the cross-plane miniband transport in n-doped [001] silicon (Si)/germanium (Ge) superlattices using an effective mass approximation (EMA) approach that correctly accounts for the indirect nature of the Si and Ge band gaps. Direct-gap based EMA has been employed to investigate the electronic properties of these superlattices; however, that does not accurately predict transport properties. We use the Boltzmann transport equation framework in combination with the EMA band analysis, and predict that significant improvement in the thermopower ($S$) of n-doped Si/Ge superlattices can be achieved by controlling the lattice strain environment in these heterostructured materials. We illustrate that a remarkable degree of tunability in the Seebeck coefficient ($S$) can be attained by growing the superlattices on various substrates and/or varying the periods and the composition of the superlattices. Our calculations show up to ~3.2-fold Seebeck enhancement in Si/Ge [001] superlattices over bulk silicon in the high-doping regime, breaking the Pisarenko relation. And the thermopower modulations lead to an increase in the power factor, $S^2\sigma$, by up to 20%, where $\sigma$ is the electronic conductivity. Our approach is generally applicable to other superlattice systems, such as to investigate the electronic transport properties of two-dimensional nanowire and three-dimensional nanodot superlattices. A material with high $S$ potentially improves the energy conversion efficiency of thermoelectric applications, and additionally is highly valuable in various Seebeck metrology techniques including thermal, flow, radiation, and chemical sensing applications. We anticipate that the ideas presented here will have a strong impact in controlling electronic transport in various thermoelectric, optoelectronic, and quantum-enhanced heterostructured materials applications.

Key words: Semiconductor superlattices, n-doping indirect-gap materials, effective mass approximation, thermopower, electronic power factor, strain, temperature

INTRODUCTION

Dimensionally confined semiconductor heterostructures, such as quantum wires, superlattices, and quantum dots, have been demonstrated to exhibit remarkable tunability of electronic and thermal transport properties, and thus offer great promises for energy transport applications. Consequently, heterostructured materials are actively being investigated to enable efficient and green energy transport and conversion applications, and to meet the increasing energy demands imposed by various modern-day devices. The intriguing transport properties observed in these materials have been mainly attributed to the presence of unique features in their density of energy states, distinguished from the corresponding bulk material characteristics. Among various
heterostructures studied, silicon (Si)/germanium (Ge)-based heterostructures are of high technological relevance due to the applications in the fields of electronics\textsuperscript{13,14} optoelectronics\textsuperscript{15–19} photonics\textsuperscript{20–22} thermoelectrics\textsuperscript{23–25} and quantum materials\textsuperscript{26–29} to name a few. With the advancements in nanofabrication techniques\textsuperscript{30,31}, it is now possible to achieve remarkable control over the growth process of the Si/Ge heterostructures\textsuperscript{32–34}. Therefore, to address the ever-growing need for efficient and green energy conversion, it is imperative to acquire a fundamental understanding of the transport properties of Si/Ge heterostructures, particularly aimed at their thermoelectric applications.

A thermoelectric material converts energy at its peak efficiency when the figure of merit, \( ZT = S^2\sigma T/\kappa \), is maximized, where \( S \) is the thermopower or the Seebeck coefficient, \( \sigma \) is the electrical conductivity, \( \kappa \) is the total thermal conductivity, and \( T \) is the absolute temperature. In recent years, \( ZT \) of Si-Ge systems has been reported to take a leap due to the introduction of nanostructuring approach. \( ZT = 1.5\)\textsuperscript{35} and 0.95\textsuperscript{36} were predicted at ~900°C for n-type and p-type SiGe alloys, respectively, grown with ball-milling techniques. These synthesis techniques introduce nanoscale features in the materials, creating a high density of interfaces or grain boundaries within the bulk. These features favorably lower \( \kappa \), mainly due to the presence of strong phonon scattering at the boundaries. In fact, engineering phonons through nanostructuring to improve the \( ZT \) of thermoelectric materials is a highly active area of research. Several approaches are being pursued, including dimensional modification in the form of one-dimensional nanowires\textsuperscript{37–39}, or two dimensional silicene\textsuperscript{40} layered graded \( \text{Si}_x\text{Ge}_y/\text{Si} \) superlattices\textsuperscript{41}, Si-Ge nanomeshes\textsuperscript{42}, or the introduction of some form of defects, such as dislocations\textsuperscript{43}, etc. In comparison, the electronic transport properties \( (S, \sigma) \) of these materials have received little attention. For example, \( S \) displays an interesting non-monotonic trend with increasing temperature in the nanostructured SiGe alloy studied in Bathula et al.\textsuperscript{35} but no attempt was made to explain the observation. More often, the electronic properties are measured experimentally or assumed to remain invariant. It is desirable to improve the factor \( S^2\sigma \), known as the electronic power factor (PF), in order to further improve \( ZT \).\textsuperscript{44} In fact, enhancing \( S \) has been reported to enhance the PF of semiconductor superlattices\textsuperscript{45}. In addition to improving the energy conversion efficiency, a material with high \( S \) is advantageous in various Seebeck metrology techniques including thermal, flow, radiation, and chemical sensing applications\textsuperscript{45,46}. Therefore, it is beneficial to discover approaches to improve the thermopower and the PF of heterostructured materials for various technological applications.

In a seminal paper, Koga et al.\textsuperscript{5} introduced the carrier pocket engineering (CPE) concept that the PF of the Si/Ge superlattices could be improved by varying the electronic properties of the well and the barrier regions, leading to significantly improved \( ZT \). The theoretical analysis in this study\textsuperscript{5} was carried out employing a Kröning–Penney (KP)-type model that ignored the indirect nature of the Si and Ge electronic band gaps. And no details were provided regarding the electronic bands of the superlattices, thermopower contributing to the improved \( ZT \), or the trade-off that exists between improvement in \( S \) and decrease in \( \sigma \) in these systems. In this article, we present our theoretical predictions of the cross-plane \( S \) of \( n \)-doped \{001\} Si/Ge superlattices, and the trade-off between \( S \) and \( \sigma \) along with its implications for the PF. We compute the miniband dispersion of these superlattices, accounting for the indirect nature of the Si and Ge band gaps by using an indirect-gap-based effective mass approximation (EMA) model\textsuperscript{44,47–49} as opposed to past KP model studies.\textsuperscript{5,50} From the miniband dispersions obtained, we employ the Boltzmann transport equation framework with constant relaxation time approximation to show that the cross-plane \( S \) of various Si/Ge superlattices can be modulated by varying strain, period, and composition. We show that the Pisarenko relation for \( S \) is broken not only by inducing substrate strain in the superlattices, but also by varying the period and composition of strain-symmetrized superlattices. We predict up to ~3.2-fold enhancement of the cross-plane \( S \) in the high-doping regime when compared to the bulk Si. Additionally, \( S \) of these superlattices shows a non-monotonic behavior with \( T \) in the low-doping regime. This indicates that \( ZT \) may not monotonically increase with \( T \) as is expected for Si/Ge superlattices. We focused on \( n \)-doped Si/Ge superlattices since we observed that their thermoelectric properties exhibit a remarkable strain dependence, although thermoelectric devices use both \( n \)-doped and \( p \)-doped materials, connecting them in series. The number of studies reporting thermoelectric properties of \( p \)-doped Si/Ge superlattices, especially using theoretical approaches, are fairly limited.\textsuperscript{10} We anticipate that \( p \)-doped \{001\} Si/Ge superlattices will also exhibit strain-, period-, and composition-dependent electronic transport properties given their strongly strain-dependent heavy and light hole band edges and effective masses.\textsuperscript{50} However, this discussion is beyond the scope of this article.

The primary advantage of our EMA-based approach is that it is much faster than other high-accuracy methods, such as density functional theory (DFT), especially for larger systems, and it helps us to form preliminary intuition about the systems considered. We presented here a comparison between the miniband dispersions predicted by the

\textsuperscript{4} All instances of increase and decrease in \( S \) mentioned in the manuscript correspond to an increase and decrease in \( \text{dS}/\text{dT} \).
EMAs and those predicted by the DFT, and concluded that the EMA is able to capture the distinguishing features fairly well. In two recent articles featuring primarily results obtained with DFT, \textsuperscript{51,52} we have shown that the thermopower obtained using the EMA bands show a similar tunability displayed by the DFT results as well. In the present article, we provide step-by-step details about the EMA approach and a discussion about the strengths and weaknesses of this approach. Our aim is to provide a comprehensive report of the EMA approach applied to the indirect-gap semiconductor superlattices. One could argue that a general theoretical framework can be constructed to treat multi-interface nanostructured systems based on the report we presented in this article along with the discussion presented in a recent publication, highlighting the effectiveness of the EMA applied to nanostructures. \textsuperscript{53} The framework will then prove to be highly beneficial to model complex Si/Ge systems, such as those investigated in Bathula et al. \textsuperscript{35} and Joshi. \textsuperscript{36}

**METHOD**

We derive the analytical dispersion relations of the [001] Si/Ge superlattice energy bands employing the EMA, also known as the envelope function approximation. \textsuperscript{44,47,48} In the EMA, the superlattice energy band dispersion relations are determined using the bulk parameters of its constituents and the band offsets. Previous studies that used EMA to compute energy bands of the Si/Ge superlattices used KP-like models that accounted for the correct superlattice band gap values; however, they ignored the indirect nature of the Si and Ge \( \Delta \) valleys, and did not account for the accurate degeneracy of the strain-split \( \Delta \) valleys to compute the total density of states. \textsuperscript{5,59} Ignoring the indirect/multi-valleyed nature of the conduction band minima (CBM) directly affects the predictions of the superlattice transport properties, since the total density of states did not include the contribution from all the degenerate valleys. The idea of using an envelope function for indirect valley states has been explored by researchers in various degrees of complexity. \textsuperscript{39,58} Here, we follow the multi-valley band structure analysis method presented by Mukherji and Nag \textsuperscript{59} in our EMA implementation to account for the indirect nature of the Si and Ge CBM. We would like to point out that this approach is very similar to using an envelope function for the \( \Gamma \) centered valleys, with the main difference being that the Bloch functions of the electrons from the indirect valleys have an offset in the crystal momenta. However, extra care must be taken to identify the superlattice momenta that correspond to a given energy, and also to account for the correct degeneracy of the strain-split \( \Delta \) valleys when considering these indirect valley states. We use the superlattice bands obtained with the EMA to compute the electronic transport properties using the Boltzmann transport equation (BTE) within the constant relaxation time approximation. We acknowledge that the tight-binding description offers an alternative approach to model the behavior of these systems (see e.g. Neophytou \textsuperscript{55} and Fiedler\textsuperscript{56}). However, we find that EMA is much simpler to implement and obtain preliminary results that would reveal interesting trends, and compares reasonably well in comparison with higher-accuracy methods, such as DFT. Additionally, a recent article discussed the reasons for the effectiveness of the EMA applied to nanostructures, \textsuperscript{53} thus providing further justification for the choice of the EMA for our investigation.

**Analytical Dispersion Relations of Si/Ge Superlattice Bands Using Effective Mass Approximation**

**Conduction Bands**

It is well known that the 6-fold degenerate \( \Delta \) valleys form the Si CBM, while the 4-fold degenerate \( \bar{L} \) valleys form the Ge CBM. \textsuperscript{57} However, the miniband energy levels from the \( \bar{L} \) valley states are much higher than those from the \( \Delta \) valleys in [001] Si/Ge superlattices. \textsuperscript{5} As a consequence, the electronic transport in \( n \)-doped [001] Si/Ge superlattices is dominated by the \( \Delta \) valley states. \textsuperscript{5} We derive the conduction miniband dispersion (CMB) of the \( \Delta \) valley states using EMA. It is necessary to identify the lattice spacings and the superlattice potential profiles to obtain the miniband dispersion relations. In relaxed configurations, Si and Ge lattice constants are \( a_{\text{Si}} = 5.431 \text{Å} \) and \( a_{\text{Ge}} = 5.658 \text{Å} \), respectively. \textsuperscript{58} In a strain-symmetrized (SS) superlattice, both the Si and Ge components are strained due to this lattice mismatch. Additionally, superlattices are usually grown on substrates which can induce further strain. We compute the lattice parameters of the SS and the substrate-strained superlattices using the macroscopic elastic energy minimization approach. \textsuperscript{59} We assume that the in-plane lattice constants of both the constituents of a substrate-strained superlattice are matched to the substrate lattice constant \( a || \). The cross-plane lattice constants of the components are given by \( a_{\perp} = a_i [1 - D_{[001]}(a_i/a_i - 1)] \), where \( a_i \) represents unstrained lattice constants with \( i = \text{Si}, \text{Ge} \), and \( D_{[001]} \) are constants depending on the elastic moduli, with \( D_{[001]} = 0.776 \) and \( D_{[001]} = 0.751 \). \textsuperscript{60} The in-plane and cross-plane strain in the superlattices are defined as \( \epsilon_{i \perp} = (a_{i \perp}/a_i - 1) \) and \( \epsilon_{i \parallel} = (a_{i \parallel}/a_i - 1) \), respectively. \textsuperscript{59} In this article, we investigate SS superlattices with varied period and composition, and the superlattices grown on substrates that induce in-plane strains in Si and Ge, in a range of \( \epsilon_{\text{Si} ||} = 0 - 4.2\% \) (tensile) and \( \epsilon_{\text{Ge} ||} = 0 - 4\% \) (compressive), respectively. \textsuperscript{50,59} We assume that the
interfaces are smooth and the superlattices are periodic in the in-plane directions.

The strain in the components splits the 6-fold degenerate Δ valleys of unstrained Si and Ge into 2-fold degenerate Δi valleys and 4-fold degenerate Δj valleys. We compute the strain-controlled potential profiles of the Δi and Δj valleys in each material using the deformation potentials of bulk Si and bulk Ge. We acknowledge that similar to each other, with effective masses of the Si and Ge

\[ E_{\parallel} + E_{\perp} = \left( \frac{\hbar^2}{2m_t} (k_x^2 + k_y^2) + V_{\text{Si}} + \frac{\hbar^2}{2m_t} (k_y^2 + k_z^2) \right) + V_{\text{Ge}} + \frac{\hbar^2}{2m_t} (k_x^2 + k_z^2) \]  

with \( V_{\text{Si}} = -0.049 \times \epsilon_{\text{Si}} + 0.373 \) and \( V_{\text{Ge}} = -0.056 \times \epsilon_{\text{Si}} + 1.157 \), and from the in-plane Δi valleys centered at (±kxo, 0, 0) as

\[ E_{\parallel} + E_{\perp} = \left( \frac{\hbar^2}{2m_t} (k_x^2 + k_z^2) + V_{\text{Si}} + \frac{\hbar^2}{2m_t} (k_y^2 + k_z^2) \right) + V_{\text{Ge}} + \frac{\hbar^2}{2m_t} (k_x^2 + k_y^2) + \frac{\hbar^2}{2m_t} (k_x^2 + k_z^2) \]

with \( V_{\text{Si}} = 0.110 \times \epsilon_{\text{Si}} + 0.373, \) and

\[ V_{\text{Ge}} = 0.094 \times \epsilon_{\text{Si}} + 0.527. \]  

A similar energy balance equation can be written for Δi valleys centered at (0, ±kxo, 0) by replacing \( k_x, k_z, k_y \) in Eq. 2 with \( k_x, k_{y0}, k_z \), respectively. The terms contributing to \( E_{\parallel} \) are collected in the curly brackets, and the rest of the terms contribute to \( E_{\perp} \). It can be clearly seen that the in-plane energy \( E_{\parallel} \) terms within the curly brackets in Eqs. 1 and 2 are identical in Si and Ge regions. This allows us to solve for the allowed \( E_{\parallel} \) in the superlattices corresponding to the six pairs of Δ valleys, independent of \( E_{\parallel} \). We note that the Δi valleys obey C2 rotational symmetry about the [100] and [010] axes, while the Δj valleys obey C4 rotational symmetry about the [001] axis. Owing to these symmetry considerations, it suffices to solve for \( E_{\parallel} \) corresponding to any one pair of valleys from each type of Δi or Δj valleys. Here, we choose to solve for the dispersion relations of the allowed \( E_{\parallel} \) states corresponding to the Δi valleys centered at (0, 0, kxo), and the Δj valleys centered at (kxo, 0, 0).

In order to obtain the analytical dispersion relations, we analyze the electronic wave functions for the allowed \( E_{\parallel} \) states of the superlattice. The in-plane translational symmetry and momentum conservation allow us to separate the wave function envelopes into in-plane \( e^{i(k_x x + k_y y)} \) and cross-plane \( \psi_j(x) \) components, with \( i = \text{Si or Ge} \) and \( j = \perp \) or \( \parallel \), respectively. The EMA or the envelope function approximation further allows us to write \( \psi_j(x) \) in the Si and Ge regions as a linear combination of their bulk Bloch states. Solving Eq. 1 for \( k_{\text{Si}} \) and \( k_{\text{Ge}} \), we find that the Bloch states at the allowed \( E_{\parallel} \) states for the Si and Ge Δi valleys correspond to
\[ k_{\text{Si}} = k_{z0} \pm K \quad \text{and} \quad k_{\text{Ge}} = k_{z0} \pm iQ, \text{with} \]
\[ K = \sqrt{\frac{2m_i(E_i - V_{\text{Si}}^i)}{\hbar^2}} \quad \text{and} \quad Q = \sqrt{\frac{2m_i(V_{\text{Ge}}^i - E_i)}{\hbar^2}}, \]
respectively. Therefore, the cross-plane wave functions from the \( \Delta \parallel \) valley states can be written as
\[ \psi_{\text{Si}}^\perp(z) = A_{\text{Si}}^\perp e^{i(k_{zi} - K)z} + B_{\text{Si}}^\perp e^{i(k_{zi} + K)z} \]
\[ \psi_{\text{Ge}}^\perp(z) = A_{\text{Ge}}^\perp e^{i(k_{jz} - Q)z} + B_{\text{Ge}}^\perp e^{i(k_{jz} + Q)z}, \]
\[ \forall E_i \geq V_{\text{Si}}^i. \] Similarly, using Eq. 2, the Bloch states at \( E_i \) for the \( \Delta \parallel \) valleys correspond to
\[ k_{\text{Si}} = \pm K \quad \text{and} \quad k_{\text{Ge}} = \pm iQ, \text{with} \]
\[ K = \sqrt{\frac{2m_i(E_i - V_{\text{Si}}^i)}{\hbar^2}} \quad \text{and} \quad Q = \sqrt{\frac{2m_i(V_{\text{Ge}}^i - E_i)}{\hbar^2}}, \]
respectively. Therefore, cross-plane wave functions from the \( \Delta \parallel \) valley states can be written as
\[ \psi_{\text{Si}}^\parallel(z) = A_{\text{Si}}^\parallel e^{-iKz} + B_{\text{Si}}^\parallel e^{iKz} \]
\[ \psi_{\text{Ge}}^\parallel(z) = A_{\text{Ge}}^\parallel e^{-iQz} + B_{\text{Ge}}^\parallel e^{iQz}, \]
\[ \forall E_i \geq V_{\text{Si}}^\parallel. \] The coefficients \( A_i^j \) and \( B_i^j \) with \( i = \text{Si or Ge} \) and \( j = \perp \) or \( \parallel \) are determined by imposing necessary boundary conditions on \( \psi_i^j(z) \). Within the EMA framework, the wave function and its derivative need to obey the Bastard continuity conditions at the interface.\(^{44}\) Additionally, the wave function needs to satisfy the Bloch condition, yielding \( \psi_i^j(z + a) = e^{iqa} \psi_i^j(z) \) and \( \psi_i^j(z + a)' = e^{iqa} \psi_i^j(z)' \) for a superlattice with period \( a \) and the cross-plane wave vector \( q \). Applying these conditions leads us to the dispersion relations of the \( \Delta \perp \) valley states centered at \((0, 0, k_{z0})\) as
\[ \cos \left((q - k_{z0})a\right) = \frac{Q^2 - K^2}{2KQ} \left(\sin (Kb) \sinh (Q(a - b))\right) \]
\[ + \cos (Kb) \cosh (Q(a - b)), \] and of the \( \Delta \parallel \) valley states as
\[ \cos (qa) = \frac{Q^2 - K^2}{2KQ} \left(\sin (Kb) \sin (Q(a - b))\right) \]
\[ + \cos (Kb) \cosh (Q(a - b)), \]
where \( a \) is the superlattice period, \( b \) the well width, and \((K, Q)\) determined from Eqs. 3 and 5, respectively. We solve Eqs. 7 and 8 numerically to obtain the \( E_{\perp} \) vs. \( q \) relationship by varying \( K \) and \( Q \) (as a function of \( E_{\perp} \), Eq. 3, and Eq. 5) and solving for \( q \). The cross-plane energies \( E_{\parallel} \) for \( \Delta \perp \) and \( \Delta \parallel \) valleys thus obtained are superposed with their corresponding \( E_{\perp} \), shown in Eqs. 1 and 2, for various \((k_x, k_y)\) to obtain the total dispersion \( E \) versus \((q, k_x, k_y)\) across the first Brillouin zone (FBZ).

**Valence Bands**

Thus far we have only discussed the dispersion relations of the conduction minibands of Si/Ge superlattices. This is because the electronic transport in \( n \)-doped Si/Ge superlattices is mainly contributed by the electrons within a narrow region around \( E_F \), usually located within the CMB energy window. The superlattices we consider in our study have a high enough band gap that the valence miniband (VMB) states do not lie in this region. As a result, theoretical predictions of electronic properties in \( n \)-doped Si/Ge superlattices include only the CMB and ignore the contribution from the VMB.\(^{5}\) Nevertheless, for the sake of presenting a complete analysis of the electronic bands of Si/Ge superlattices using EMA, we briefly discuss the derivation of VMB dispersion relations considering a simplified model for the anisotropic heavy holes (IH) and light holes (LH) of Si and Ge. Similar to the \( \Delta \) valley case, it is important to correctly account for the potential profiles and the effective masses of the HH and LH in the Si and Ge regions of the superlattice. The valence band maxima (VBM) of LH and HH coincide at the \( \Gamma \) point for unstrained Si and Ge and undergo degeneracy lifting under strain. We compute the strain-controlled LH and HH potential profiles of Si and Ge in a [001] Si/Ge superlattice using the deformation potential theory.\(^{59}\) We denote the strain-split HH and LH VBM with \( V_j^i \) with \( i = \text{Si or Ge} \) and \( j = \text{HH or LH} \), respectively. The FS of HH and LH are ellipsoids centered at the \( \Gamma \) point with longitudinal and transverse effective masses that have nonlinear strain dependence.\(^{64-66}\) We assume that the HH effective masses are strain-independent, with longitudinal effective masses \( m_{\text{HH}}^\text{Si} = 0.28m_0 \) and \( m_{\text{HH}}^\text{Ge} = 0.22m_0 \), and transverse effective masses \( m_{\text{HH}}^\text{Si} = 0.22m_0 \) and \( m_{\text{HH}}^\text{Ge} = 0.06m_0 \) for the sake of simplicity. On the other hand, we assume that the LH longitudinal effective masses decrease linearly from 0.20\( m_0 \) to 0.18\( m_0 \) for Si \((m_{\text{LH}}^\text{Si})\) and increase from 0.05\( m_0 \) to 0.14\( m_0 \) for Ge \((m_{\text{LH}}^\text{Ge})\).\(^{50}\) to the lowest to highest strain experienced by Si (tension) and Ge (compression), respectively. We assume that the LH transverse effective masses are strain-independent at \( m_{\text{LH}}^\text{Si} = 0.25m_0 \) and \( m_{\text{LH}}^\text{Ge} = 0.07m_0 \).
With the effective masses characterized, we can write the energy conservation of the HH states across the interface as

$$E = V_{HH}^{Si} + \frac{\hbar^2 k_x^2}{2m_{HH}^{Si}} + \left\{ \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_{HH}^{tSi}} \right\}$$

$$= V_{HH}^{Ge} + \frac{\hbar^2 k_x^2}{2m_{HH}^{Ge}} + \left\{ \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_{HH}^{tGe}} \right\},$$

(9)

with $V_{HH}^{Si} = 0.003 \times \epsilon_{Si} - 0.778$ and $V_{HH}^{Ge} = 0$. A similar relation can be written for the LH state, replacing the HH effective masses with that of the LH in Eq. 9, with $V_{HH}^{LH} = 0.099 \times \epsilon_{Si} - 0.778$ and $V_{HH}^{LH} = 0.004 \times \epsilon_{Ge}^2 + 0.009 \times \epsilon_{Si} - 0.149$. 50, 59 We note that the in-plane energy components in Si and Ge regions shown in the curly brackets in Eq. 9 are not similar to each other, unlike the $\perp$ valley case, due to the difference in the transverse effective masses. Therefore, the total energy $E$ cannot be split into $E_{\perp}$ and $E_{\parallel}$ components. We solve for the allowed $E$ vs. $(q, k_x, k_y)$ employing EMA for various total in-plane momenta $k_{\parallel}$. Here, the $E$ at a given $q$ and $k_{\parallel}$ corresponds to all possible $(k_x,k_y)$ pairs that satisfy the chosen $k_{\parallel}$. By choosing various $k_{\parallel}$, we compute the VMB across the FBZ in a manner similar to the CMB. For a rigorous calculation of the VMB, including a full consideration of the anisotropy and the strain dependence of the hole effective masses, the reader is advised to consult other references. 64–66 These studies provide particularly useful insight for analyzing electronic transport in $p$-doped Si/Ge superlattices employing the EMA.

First-Principles Energy Dispersion Relations of Si/Ge Superlattice Bands

In order to establish the reliability of transport property predictions using EMA, it is important to understand how the EMA bands compare to those obtained with a higher-accuracy numerical method. We compare the EMA bands of strained Si$_4$Ge$_4$ superlattices with those obtained with DFT (Fig. 1). The electronic structure properties are obtained using the plane-waves code Quantum Espresso (QE). 67 Our Si$_4$Ge$_4$ model superlattice supercell consists of four and eight monolayers (MLs) in the in-plane and cross-plane directions, respectively, and corresponds to a tetragonal Brillouin zone. To simulate the effect of substrate strain, we fix the in-plane lattice constant $a_{\parallel}$ corresponding to the substrate lattice constant, inducing the in-plane strain $\epsilon_{Si,||}$. We then relax the superlattice in the [001] cross-plane direction by performing a self-consistent field (SCF) calculation using the Broyden–Fletcher–Goldfarb–Shanno quasi-Newton algorithm. The SCF calculations are performed on a $4 \times 4 \times 2$ $k$-mesh using the generalized gradient approximation (GGA) of the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional by employing scalar relativistic norm-conserving pseudopotentials for Si and Ge atoms. 68 We generate the $k$-mesh employing the Monkhorst–Pack scheme, which reduces the computational time significantly owing to the superlattice symmetry. 69 An energy cutoff of 30 Ry was used to expand the Kohn–Sham orbitals in terms of a plane-wave basis set. 65, 67 A convergence threshold of $10^{-9}$ Ry was used for self-consistency. Following the SCF calculations, we perform the electronic structure calculations for the Si$_4$Ge$_4$ superlattice using non-self-consistent field (NSCF) calculations. We use a dense $k$-mesh of $40 \times 40 \times 20$ for all our NSCF calculations. We ignore the spin–orbit (SO) coupling effects in our analysis, since it was shown that the strain splittings of the bands are much larger than the SO splittings. 71

Electronic Transport Coefficients Using the Boltzmann Transport Equation

We use BTE with the constant relaxation time approximation to compute the electronic transport properties of $n$-doped Si/Ge superlattices. Specifically, the cross-plane Seebeck coefficient $S$ and the electrical conductivity $\sigma$ are obtained using the following expression: 57, 72

$$L^{(a)} = \tau \int dE \left[ \frac{\partial^2 \rho_{DOS}(E)}{\partial E^2} \right]$$

(10)

$$\sigma = L^{(0)}$$

(11)

$$S = \frac{1}{eT} L^{(1)}$$

(12)

where $e$ is electron charge, $T$ is temperature, $\tau$ is the electron relaxation time, $E$ is energy, $v_g(E)$ is the average cross-plane group velocity of an electron with energy $E$, $\rho_{DOS}(E)$ is superlattice density of states (DOS), $E_F$ is the Fermi level, and $f_0(E)$ is the Fermi–Dirac distribution function. In order to compute the $S$ and the $\sigma$ as a function of the carrier...
concentration $n_e$, we employ the following relation.\textsuperscript{9,73}

$$n_e = \int dE \rho_{DOS}(E)f_0(E). \quad (13)$$

## RESULTS

We now discuss our main results demonstrating various band-engineering approaches to modulate the thermopower and the other electronic transport coefficients of n-type Si/Ge superlattices using EMA.

### Comparison Between Energy Bands Obtained with Different Methods

We show the comparison between the energy bands of substrate-strained Si$_4$Ge$_4$ superlattices computed with EMA and DFT in Fig. 1 to establish the predictive power of the EMA. The respective substrate induced in-plane strain values are shown at the bottom of the figure. The EMA models are chosen to represent superlattices with $\varepsilon_{Si} = \{0.7\%, 2.1\%, 3.5\%\}$. We compare the band structures of these EMA models with the DFT models representing $\varepsilon_{Si} = \{0.8\%, 2.4\%, 4.0\%\}$. As can be noted, the strain values as well as the lattice parameters do not have a one-to-one comparison between the two methods. The unstrained Si and Ge lattice constants predicted by DFT and EMA are $a_{Si}^{DFT} = 5.475 \, \text{Å}$, $a_{Ge}^{DFT} = 5.740 \, \text{Å}$ and $a_{Si}^{EMA} = 5.431 \, \text{Å}$, $a_{Ge}^{EMA} = 5.658 \, \text{Å}$, respectively. The in-plane strain in confined Si, $\varepsilon_{Si}$, of the superlattice DFT models grown on a Si or a Ge substrate ranges from 0% to 4.8%, respectively. This is in contrast to the respective 0–4.2% range present in the EMA models. To establish a common reference for comparison, we scale the EMA-predicted $\varepsilon_{Si}$ in the 0–4.2% range to fit within the DFT-predicted 0–4.8% range, and estimate the strain in an equivalent DFT model. We further align the Fermi levels ($E_F$) of the EMA and DFT bands and set them to 0 eV to facilitate the band structure comparison. We note that the splitting of $\Delta$ valleys and their strain-induced relative movements are very well predicted by both the DFT and the EMA approaches. However, EMA models consider a larger band gap compared to DFT, which leads to a misalignment of the minibands. This happens because of the systematic underestimation of the band gaps by the Kohn–Sham states in the DFT.\textsuperscript{74} The PBE functional, in particular, predicts an incorrect 0 eV band gap for Ge.\textsuperscript{75} While in the EMA, we correctly account for the band gaps of unstrained Si and Ge by matching them with their experimental values of $\sim 1.17 \, \text{eV}$ and $\sim 0.96 \, \text{eV}$, respectively.\textsuperscript{59,76} Therefore, one needs to adjust the DFT bands shown in Fig. 1 with the correct band gaps to show a better overall match between the EMA and DFT band structures. Nevertheless, the EMA and the DFT CMB match well, except that EMA does not predict sub-band splittings due to the exclusion of the inter-valley mixing effects. With the reliability of the EMA bands established by comparing with DFT, we proceed to analyze the electronic transport properties of the superlattices using these bands, which we perform at $T = 300 \, \text{K}$ unless mentioned otherwise.

### Electronic Transport Coefficients of Si/Ge Superlattices

#### Substrate-Strained Superlattices

We demonstrated that strain-induced CMB modulations enable tunable enhancements of the electronic thermopower of the Si/Ge superlattices, especially in the high-doping regime, in our recent work using DFT.\textsuperscript{51,52} Here, we aim to illustrate that such strain-controlled modulations of $S$ are also captured within a simpler EMA approach, as this further substantiates our EMA methodology and helps us to form physical intuition about the system. To this end, we compute the electronic transport coefficients of the strained Si$_4$Ge$_4$ superlattices with $\varepsilon_{Si} = \{0.7\%, 2.1\%, 2.8\%, 3.5\%, 4.2\%\}$ employing the EMA. We present the EMA-BTE-predicted $S$ of the strained superlattices and that of bulk Si in Fig. 2a(i). The $S$ of bulk Si monotonically decreases with increasing carrier concentration ($n_e$), following a Pisarenko-like relation (PR).\textsuperscript{10} The $S$ of strained Si$_4$Ge$_4$ superlattices shows a bulk-like monotonic behavior in the low-strain regime ($\varepsilon_{Si} \leq 0.7\%$), and is reduced compared to bulk Si. As we increase $\varepsilon_{Si}$, we note the emergence of an oscillatory behavior as a function of the carrier concentration $n_e$, breaking the PR. A general trend can be noted that the peaks move towards higher $n_e$ with increasing strain. A similar trend was observed in the first-principles DFT study as well.\textsuperscript{52} Our EMA-BTE approach predicts a $\sim 2.4$-fold enhancement of $S$ at $n_e = 5.2 \times 10^{20} \, \text{cm}^{-3}$ for a substrate-strained Si$_4$Ge$_4$ superlattice with $\varepsilon_{Si} = 4.2\%$. While enhancement of $S$ has its own advantages, it is important to characterize how the strain-induced CMB modulations affect other electronic transport coefficients, to use the strain engineering approach for a broad range of technological applications including thermoelectric applications.

We present the variation of $\sigma$ and PF (in the units of $\tau$) of strained Si$_4$Ge$_4$ superlattices with $n_e$ in Figs. 2a(ii) and (iii), respectively. The $\sigma/\tau$ of bulk Si increases monotonically with increasing $n_e$, compensating for the monotonic decrease in the $S$. This $S - \sigma$ trade-off results in the PF peak at $n_e \sim 3.2 \times 10^{20} \, \text{cm}^{-3}$, in a similar manner as discussed in previous studies.\textsuperscript{10} Interestingly, $\sigma$ of Si$_4$Ge$_4$ superlattices is slightly increased in the low-strain (0.7%) regime, compensating for the decrease in $S$. As a result, the PF peak shifts towards lower $n_e$ resulting
in a \( \sim 10\% \) increase in PF for \( n_e < 5 \times 10^{19} \text{ cm}^{-3} \). However, \( \sigma \) is reduced in the superlattices with moderate (2.1\%) to high (4.2\%) substrate strain. This results in a reduced PF for \( n_e < 10^{20} \text{ cm}^{-3} \) for moderate- to high-strain cases. A trend can be noted that the PF peak becomes sharper and shifts towards higher \( n_e \) with increasing strain. PF is \( \sim 20\% \) improved at \( n_e \sim 11 \times 10^{20} \text{ cm}^{-3} \) for the highest-strain case (4.2\%). This re-establishes the idea that the miniband modifications induced by the substrate strain can help modulate electronic transport in superlattices.

**Strain-Symmetrized Superlattices with Varied Period**

However, it was found that it is energetically unfavorable to grow strained Si/Ge superlattices.\(^{77-80}\) Instead, SS superlattices are more stable and can be grown easily.\(^{79}\) In these superlattices, strain originates due to the lattice mismatch between the superlattice components. Hence, it is of practical interest to explore the strain-induced electronic properties of SS superlattices. Previous studies reported that the electronic transport in the SS superlattices can be modulated by varying the superlattice periods and the layer thicknesses.\(^{9,10,77,81,82}\) In Fig. 2b, we present the electronic properties of SS Si\(_n\)Ge\(_n\) superlattices with varied periods, \( L = 2n \), where \( n = \{5, 10, 16, 22, 32\} \) MLs. Interestingly, the in-plane strain in the confined silicon components of the SS superlattices is a constant, \( \epsilon_{\text{Si,\parallel}} = 1.9\% \), independent of \( n \).\(^{89}\) Since the \( \epsilon_{\text{Si,\parallel}} \) is the same for all the chosen superlattices, the potential profiles in Si and Ge regions are also the same. The only variables are the widths of the Si (well) and Ge (barrier) regions, which vary by the same number of MLs, resulting in the variation of the period of the superlattice. We predict that these superlattices display an oscillatory \( S \) with respect to \( n_e \) as shown in Fig. 2b(i), breaking the PR. Particularly, the \( n = 10, 16, \) and 22 superlattices show a strong oscillatory behavior with regions of increase and decrease in \( S \). While the \( n = 5 \) and 32 superlattices show an increased \( S \) for all \( n_e \) considered, with the \( n = 32 \) superlattice showing a remarkable increase in overall \( S \). The thermopower of the \( n = 32 \) superlattice shows a maximum \( \sim 3.2\text{-fold} \) enhancement at \( n_e = 7 \times 10^{19} \text{ cm}^{-3} \). However, the increase in \( S \) is compensated by the decrease in \( \sigma \) as shown in Fig. 2b(ii), in a similar manner as that of the substrate-strained superlattices discussed before. This \( S - \sigma \) trade-off results in the drastically diminishing PF for \( n_e < 10^{20} \text{ cm}^{-3} \), as shown in Fig. 2b(iii). On the other hand, in the high-doping regime \( n_e > 5 \times 10^{20} \text{ cm}^{-3} \), we observe a 10–20\% enhancement of PF for \( n = 5, 16, \) and 22 superlattices. Through this analysis, we establish that modulations in the electronic transport properties can be achieved by varying the period of the SS Si/Ge superlattices.
Strain-Symmetrized Superlattices with Fixed Period and Varied Composition

The strain-symmetrized superlattices we have discussed thus far have a constant potential profile owing to the equal number of Si and Ge MLs. However, the strain in the SS superlattices varies when the number of Si (p) and Ge (q) MLs is varied independently. The nonuniform strain leads to variable potential profiles in the Si and Ge regions. Additionally, the ratio of well to barrier width is not constant in these cases. Here we investigate Si$_p$Ge$_q$ superlattices with $p + q = 32$ MLs. In Fig. 2c, we present the electronic transport properties of Si$_p$Ge$_q$ superlattices with $(p, q) = (20, 12), (16, 16), (12, 20))$ yielding symmetrized strains, and $\epsilon_{Si_{\parallel}} = (1.4\%, 1.9\%, 2.4\%)$. In Fig. 2c(ï), we find that for $p > q$, $S$ in the low-doping regime is enhanced considerably, while maintaining an overall improvement in the mid- to high-doping regimes. Increasing the Ge MLs tends to push the high-S regions to higher $n_e$ preceded by low regions in the form of oscillatory peaks. The Si$_{12}$Ge$_{20}$ superlattice shows a significant ~3-fold $S$ enhancement compared to the bulk Si at $n_e = 7 \times 10^{19} \text{cm}^{-3}$. Interestingly, among the three cases studied, the $S - \sigma$ trade-off plays in such a way that the $p = q$ case gives the maximum enhancement in the PF in the high-doping regime.

Qualitative Explanation of the Modulation of Electronic Transport in Superlattices

We demonstrated that the Pisarenko-like $S$ vs. $n_e$ inverse relationship can be broken in substrate-strained and strain-symmetrized n-doped Si/Ge superlattices. Only a few studies reported such a behavior in Si/Ge superlattices. It is therefore important to understand the mechanism that governs this behavior to aid future research. At a given temperature, $S \propto \mathcal{L}^{(1)} / \sigma$ in the BTE framework (Eq. 12). Therefore, to understand the behavior of $S$ with $n_e$, it is imperative to understand the functional relationship of $\mathcal{L}^{(1)}$ and $\sigma$ with $n_e$. We note that both $\mathcal{L}^{(1)}$ and $\sigma$ are determined from the integrals containing the product $v_g^2 \rho_{\text{DOS}}(-\frac{\partial \epsilon}{\partial E})$. The term $v_g^2 \rho_{\text{DOS}}$ can be thought of as the electronic contribution to transport at energy $E$. While the term $(-\frac{\partial \epsilon}{\partial E})$, referred to as the Fermi window (FW), determines the energy window in which the dominant electronic contribution to transport occurs. The FW is centered at and symmetric with respect to $E_F$, and reaches full width at half maximum ~3.5$k_B T$, where $k_B$ is the Boltzmann constant. As the $n_e$ is increased at a fixed $T$, the FW shifts in energy as $E_F$ increases in energy. The $\mathcal{L}^{(1)}$ integral additionally includes the product of $(E - E_F)$ and the FW, resulting in an antisymmetric window (ASW) function in the numerator. Due to the presence of the ASW in $\mathcal{L}^{(1)}$, the electrons with energy above $E_F$ contribute positively towards the net $S$ and are referred to as hot electrons, while the electrons with energy below $E_F$ contribute negatively towards $S$ and are referred to as cold electrons. This distinction between the integrands of $\mathcal{L}^{(1)}$ and $\sigma$ can be used to explain the intriguing behavior of $S$ and the $S - \sigma$ trade-off mentioned before. We present a brief discussion of this aspect in the following paragraphs to explain our observations. The interested reader is encouraged to consult previous studies to acquire more understanding of the physical phenomena.

(a) In strained Si$_4$Ge$_4$ superlattices, the minibands from the $\Delta \parallel$ valleys move upward in energy with respect to those from the $\Delta \perp$ valleys, with increasing strain, $\epsilon_{Si_{\parallel}}$. This energy shift creates an oscillatory peak in the $S$ vs. $n_e$ curve that moves towards higher $n_e$ as $\epsilon_{Si_{\parallel}}$ increases from 2.1% to 4.2% as shown in Fig. 2a. The high $n_e$ peak also narrows with increasing strain since the first $\Delta \parallel$ miniband states move closer to the second $\Delta \parallel$ miniband states as shown in Fig. 1.

(b) In strain-symmetrized Si$_p$Ge$_q$ superlattices with varied periods, we increase the well and barrier widths simultaneously. As explained before, this implies the potential profile of the $\Delta \parallel$ and $\Delta \perp$ valleys within the well and barrier regions is unaffected. Therefore, the modulation of the minibands in these superlattices is primarily due to the reduction of the BZ in the cross-plane direction. In a reduced BZ, the number of minibands is increased owing to the band folding effects. Therefore, the FW...
and ASW include more oscillations of the $v^2_{g\rho \text{DOS}}$, which manifests as a strong oscillatory $S$, especially for $n = 10, 16, 22$ superlattices. Interestingly, the oscillatory nature is less prominent in the $n = 32$ superlattice. This is because although there are more minibands in the $n = 32$ superlattice, some minibands are sufficiently close to each other that the FW and ASW cannot distinguish them as distinct bands.

(c) In strain-symmetrized Si$_p$Ge$_q$ superlattices with fixed periods, we vary the composition of the well and the barrier components keeping the total number of the MLs fixed. In all the superlattices, the period and hence the superlattice BZ is approximately invariant. Therefore, the major factors that influence the miniband dispersion are the variable symmetrized strains, and the well and barrier widths. A variable symmetrized strain, as explained previously, implies a varying potential profile in the well and the barrier regions. When $p > q$, the $a_1$ of the superlattice tends to relax close to $a_{Si}$, and the potential profiles tend towards that of the low substrate strain case. This effect, in conjunction with the increased well width, results in a sharper increase in the $v^2_{g\rho \text{DOS}}$ in the low-doping regime compared with bulk Si. This in turn leads to a considerable improvement of $S$ in the low-doping regime. On the other hand, in the case of $p < q$, the $a_1$ of the superlattice tends to relax close to $a_{Ge}$, and the potential profiles tend towards that of the high-substrate-strain case. Moreover, the barrier width is considerably increased in this case, which further narrows the minibands. These effects together lead to a sharp increase in the $v^2_{g\rho \text{DOS}}$, leading to a local $S$ peak in the high-doping regime.

**Effect of Temperature on Thermopower of Superlattices**

We have demonstrated the various ways to modulate $S$ as a function of $n_e$ at a fixed $T = 300$ K, by modifying the superlattice band structure with varied strain, period, and composition. However, the FW width varies with $T$, resulting in a temperature dependence in $S$. In degenerate semiconductors, there exists a direct relationship between $S$ and $T$ at a fixed doping level. In Fig. 3, we show a monotonically increasing $S$ vs $T$ relationship for bulk Si (dashed lines) $\forall n_e$ considered. However, we find that this monotonic relationship is broken in Si/Ge superlattices, especially at the technologically relevant doping regime. $S$ of Si$_{32}$Ge$_{32}$ superlattices increases with $T$ up to $450$ K and drops as we go higher in $T$, for $n_e < 10^{19}$ cm$^{-3}$, as shown in Fig. 3 (solid lines). This can be qualitatively explained from the understanding that the FW and hence the ASW broaden with increasing $T$, leading to a variation in the contribution from the hot and the cold electrons to $S$ with $T$ at a given $n_e$. In the case of bulk Si, the ASW broadening leads to an increased contribution from the hot electrons due to a monotonically increasing $v^2_{g\rho \text{DOS}}$, while the non-monotonic nature of the $v^2_{g\rho \text{DOS}}$ results in the observed behavior in the Si$_{32}$Ge$_{32}$ superlattice. As $T$ is increased to $450$ K, the superlattice miniband states that resulted in a bump in $S$ at $T = 300$ K around $n_e \sim 7 \times 10^{19}$ cm$^{-3}$ (Fig. 2) contribute to $S$ at a lower $n_e$ due to the ASW broadening. Therefore, we see up to ~2.4-fold $S$ enhancement at $T = 450$ K in the low-doping regime. However, a further increase in $T$ extends the ASW to include the shallow $v^2_{g\rho \text{DOS}}$ region, corresponding to the cross-plane miniband transport that follows the miniband states that led to the bump at $300$ K, resulting in a decreasing $S$. In the high-doping regime, $n_e > 3 \times 10^{20}$ cm$^{-3}$, $S$ monotonically increases with $T$, approaching a Pisarenko-like behavior as observed in bulk Si. The $E_F$ is high enough that the miniband-like nature is less apparent in the high-doping regime.

**DISCUSSION AND OUTLOOK**

We analyzed the cross-plane miniband transport in $n$-doped [001] Si/Ge superlattices with the effective mass approximation, and explored ways to enhance the electronic thermopower and the power factor. To the best of our knowledge, only direct-gap-based EMA has been employed so far to investigate the electronic transport properties of Si/Ge superlattices. Here we established a new indirect-gap-based EMA approach to correctly account for the indirect nature of the Si and Ge band gaps in the analysis. We compared the energy bands obtained with EMA with those computed with DFT to discuss the reliability of the approach. Using a BTE framework in combination with the EMA band analysis,
we revealed that $S$ of $n$-doped Si/Ge superlattices can be enhanced up to $\sim 3.2$-fold in high-doping regimes, breaking the Pisarenko relation. We demonstrated that this tunability can be achieved by growing the superlattices on various substrates and/or varying the superlattice period and the composition. The increase in $S$ is largely compensated by the decrease in $\sigma$, leading to a reduced PF in most of these cases. However, we observed modest improvement of the PF of superlattices under a low (high) substrate strain, in low (high)-doping regimes. We note improvements in the PF of symmetrically strained superlattices in the high-doping regimes as well with varying period and composition. A PF value similar to or greater than that of bulk Si could result in further improvements in the $ZT$ of nanostructured materials at various doping regimes, when combined with a reduced $\kappa$. We show that in addition to varying non-monotonically with increasing $n_d$ due to lattice strain, $S$ shows a non-monotonic increase with increasing $T$, especially in the low-doping regime. Therefore, further analysis is required to estimate the electronic transport properties of [001] Si/Ge superlattices at varied strain environments or desired temperatures. Our work can provide important insight for designing experimental studies to optimize the thermoelectric performance of these materials. For example, with a fabricated Si/Ge superlattice, an experimentalist might be able to change the doping concentration using an electrostatic doping approach and optimize the thermopower. If the probing approach yields a peak, that will confirm our numerical observation. Also, if successful, the experimentalist could grow the Si/Ge superlattice on a substrate that induces less (more) strain and find a peak thermopower at a lowered (increased) doping concentration. Similarly, an experimentalist can also anticipate that having a greater (lower) $p/q$ ratio in a Si$_x$Ge$_{1-x}$ superlattice will result in improved Seebeck coefficients at lower (higher) concentrations, in general, as shown in Fig. 2c.

Further improvements could be made in the current work by including the inter-valley mixing effects, non-conservation of transverse momentum, and a non-constant electronic relaxation time. In addition, perturbation theory may be employed in conjunction to correctly account for the band splittings at the Brillouin zone boundaries. We hope that our analyses act as preliminary predictions encouraging further theoretical and experimental research to validate our findings. Our approach can be extended to other superlattice systems as well. For instance, one can use the methods presented in this work to study the electronic transport in two-dimensional nanowire superlattices and three-dimensional nanodot superlattices. Numerical matrix method-based approaches may be employed to carry out the analysis. We anticipate that the ideas presented here will have a strong impact in controlling electronic transport in various thermoelectric, optoelectronic, and quantum-enhanced heterostructured materials applications.

ACKNOWLEDGMENTS

The work is funded by the Defense Advanced Research Projects Agency (Defense Sciences Office) [Agreement No. HR0011-16-2-0043]. All computations were performed using the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562.

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