Enhancement of thermoelectric efficiency by uniaxial tensile stress in n-type GaAs nanowires

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Abstract: **The thermoelectric power-factor (PF) and efficiency (ZT) of GaAs nanowires (NWs) can be improved by (i) choosing a proper wire growth and channel orientation and, (ii) by applying uniaxial tensile stress. In this work we study the impact of these two factors on PF and ZT. Tensile stress, channel direction and cross-section size allows bandstructure engineering to tune the electronic conductance (G) and the Seebeck coefficient (S). [110] GaAs NWs grown on (111) surface provide maximum PF (~3X) and ZT (~1.7X) compared to [100]/(100) NWs, which can be attributed to the G enhancement induced by the L valley contribution under strain.**

Index Terms – GaAs, uniaxial-stress, thermoelectricity, Tight-binding.

I. INTRODUCTION

Inherent low thermal conductivity and high electron mobility can make GaAs a promising thermoelectric material [1][2]. However, GaAs suffers from DOS bottleneck which results in low electron density [3] and hence low electronic conductivity (G). It has been shown experimentally that nanowires (NWs) can improve thermoelectric efficiency (ZT) many times over bulk material [4]. Uniaxial tensile stress can reduce DOS bottleneck in GaAs by increasing the L valley contribution [5] . Guided by these experimental observations, we conducted a theoretical study to understand the impact of ***(a)*** *channel and growth direction (X/Y) and* ***(b)*** *uniaxial strain* on the thermoelectric power factor ($PF=S^2G$) and figure of merit (ZT) [4][6] in GaAs NWs.

II. THEORY AND APPROACH

In the first step of analysis the electronic bandstructure of GaAs NWs is calculated using an atomistic 20 band sp3d5s* tight-binding (TB) model [7][8]. A new set of TB parameters optimized also for the X and L valley of GaAs has been obtained which will be published elsewhere. The value of PF depends on the electronic conductance (G) and the Seebeck coefficient (S) [6] which are calculated using Landauer's formula at a given temperature T [6][9].

NW details: Atomistic square GaAs NWs with intrinsic channel are studied with specific channel (X) and growth (Y) directions for a given width (W and height (H=W)) (Fig.1). Seven different combinations of [X]/(Y) are considered for these NWs (**Table 1**) for W ranging from 2 to 6nm. Uniaxial tensile strain values vary from 0, 1, 2, 3 to 4% along the X direction All the device terminal characteristics are calculated at T=300K.

III. RESULTS AND DISCUSSION

Uniaxial tensile stress improves the maximum thermoelectric PF as shown in Fig. 2. The maximum improvement is obtained in device IV under 4% strain (~3X) as compared to the unstrained device. Other orientations also show improvement with stress except for device II. Improvement comes from the increased contribution to G of the L valley under uniaxial tensile stress along with the Γ valley (Fig. 3) [5]. Device II degrades under increasing strain since the CB valleys making contribution to G are heavier (higher transport mass).

The value of G (for device IV) shows enhancement with strain (Fig. 4). At a constant 1D inversion charge density (N1D) the value of G increases (~1.2X) due to more bands close to the Fermi level (Ef). However, the S value stays nearly the same (~0.98X). Thus, strain improves G without degrading S too much, which enhances the maximum PF.

The thermoelectric figure of merit (ZT) is calculated at T=300K using the electronic properties obtained from Landauer's approach [9] and lattice thermal conductivity (κ_e) of 0.1W/m-K reported for 56nm GaAs NWs [1]. Uniaxial stress improves ZT for all the GaAs NWs except for device II due to the lower PF for reasons mentioned above. The maximum improvement of ~1.7X in ZT is obtained in device IV (Fig. 5). The ZT improvement is obtained at higher N1D with increasing strain (Fig. 6.a), since more bands are filled at higher strain which increases G but also slightly degrades S. The maximum ZT value increases with reduction in W for all the devices except for device IV (Fig. 6.b) due to the enhancement in PF with W scaling.

IV. CONCLUSION

The possibility of GaAs NWs to serve as the next generation thermoelectric material has been shown. A proper choice of growth and channel orientation along with uniaxial stress provides a good way to enhance both the PF and ZT of GaAs NWs. A 4% uniaxial tensile stress can improve the PF and ZT (highest value of 0.36 at 300K) by ~3X and ~1.7X, respectively in 6nm NWs which further increases with W scaling. The present study shows only the impact of strained bands on thermoelectricity excluding any scattering effects.

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Table 1: Details of the channel orientation (X) and growth direction (Y) for GaAs NWs used in this study.

NW Label	I	II	III	IV	V	VI	VII
Channel [X]	[100]	[100]	[110]	[110]	[111]	[11-2]	[11-2]
Growth (Y)	(100)	(110)	(100)	(1-11)	(-110)	(1-10)	(111)

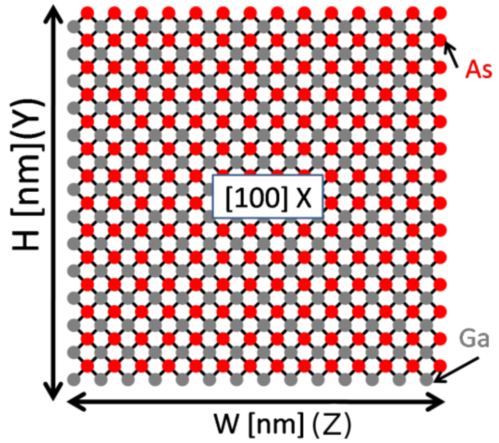

Figure 1: Projected cross-section of a GaAs nanowire (NW) along the [100] channel direction (X). The wire growth direction is along the Y axis. W (H) represents the width (height) of the NW. In this case H=W~4nm. Gray (red) dots are Ga (As) atoms.

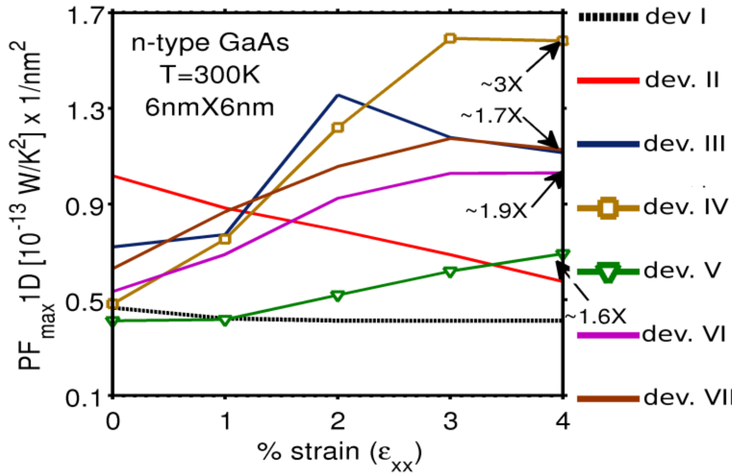

Figure 2: Variation in n-type thermoelectric maximum power factor (PF) with uniaxial tensile strain for different wire growth and channel orientations for 6nm X 6nm square GaAs NWs.

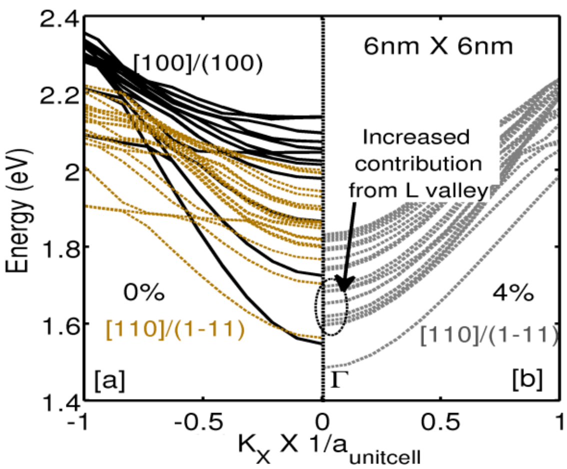

Figure 3: Conduction band E(k) for 6nm X 6nm GaAs NWs at (a) 0% and (b) 4% uniaxial stress. In the left panel E(k) for both dev. I (black) and II (brown) are shown for comparison.

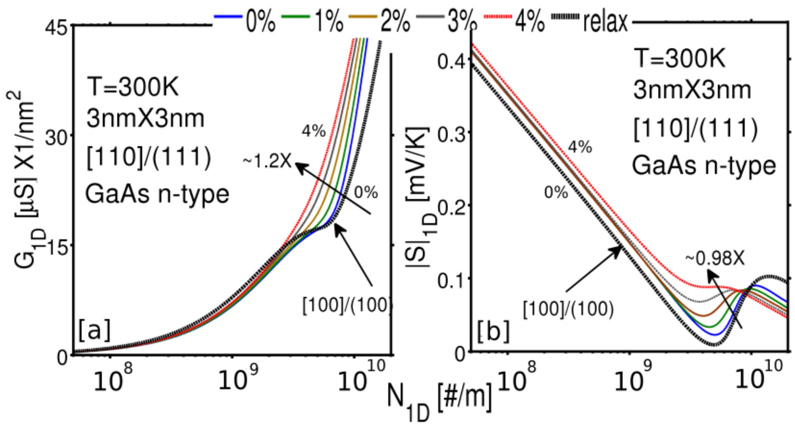

Figure 4: Variation in (a) Ballistic conductance (G) and (b) Seebeck coefficient (S) for 3nm X 3nm [110]/(111) square GaAs NW as function of N1D for various strain values. For comparison [100]/(100) GaAs NW values are also shown. The increase in G with uniaxial tensile stress is attributed to additional L valley contribution [5].

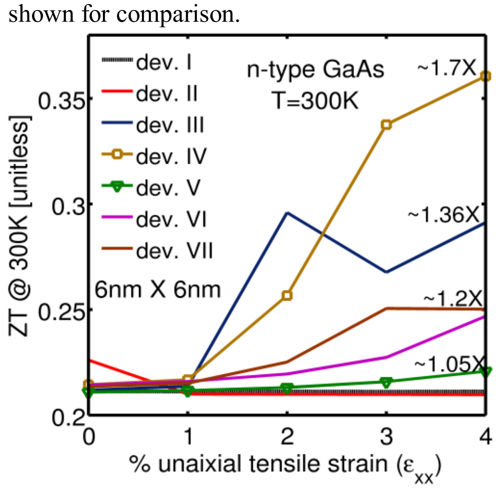

Figure 5: Variation in n-type thermoelectric power factor (PF) with uniaxial tensile strain for different wire growth and channel orientations for 6nm X 6nm square GaAs NWs.

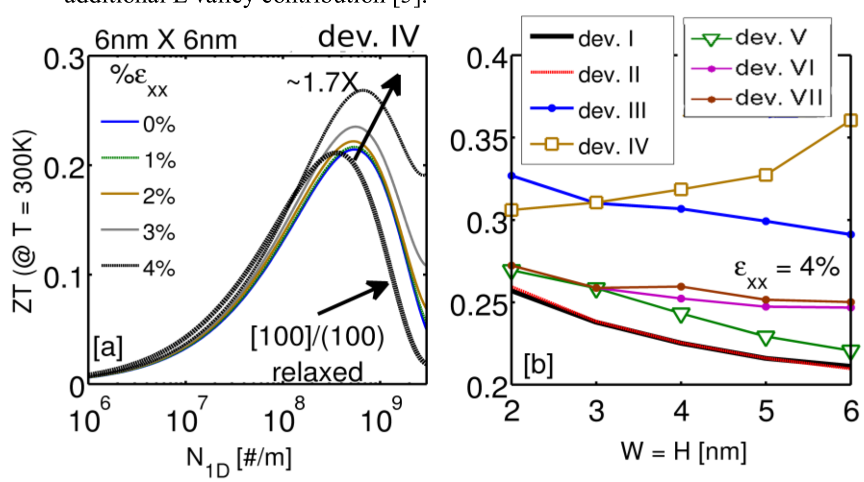

Figure 6: (a) Variation in n-type ZT of GaAs NWs at T=300K with N1D for different strain values for dev. IV with W = H = 6nm. (b) Variation in ZTmax (T=300K) with W (=H) at ε_{xx} = 4% for different devices. Device IV and III show the best ZTmax among all the configurations for various W values.