In situ mechanical resonance behaviour of pristine and defective zinc blende GaAs nanowires

Edmund Pickering,¹ Arixin Bo,¹ Haifei Zhan,² Xiaozhou Liao,³ Hark Hoe Tan⁴ and YuanTong Gu^{1*}

¹School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, 4000, Australia

²School of Computing, Engineering and Mathematics, Western Sydney University, Locked Bag 1797, Penrith NSW 2751, Australia

³School of Aerospace, Mechanical and Mechatronic Engineering, The University of Sydney, NSW 2006, Australia

⁴Department of Electronic Materials Engineering, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 2601, Australia

*Author to whom correspondence should be addressed. Email: yuantong.gu@qut.edu.au

Expanded in situ resonance methodology

In situ resonance was conducted within a dual-beam scanning electron microscope (SEM), focused ionbeam system (FEI Quanta 200 3D). The electrostatic probe (ESP) was constructed in-house and an Agilent 33500B was utilised to produce the AC/DC signal. A feedthrough was utilised to allow for the connection of the external control and measurement devices to the experimental setup within the chamber. The ESP was brought into close proximity to the target nanowire (NW) and an AC voltage (with possible DC offset) was applied to the ESP. The application of a voltage produces a charge build up on the ESP and a complimentary charge build up in the target NW, producing an electrostatic force. Thus, through this technique, a cyclic voltage applied to the ESP via the function generator produces a cyclic force of controllable frequency (ranging from 1 Hz to 20 MHz) and magnitude. This allows for fine control of the forcing frequency across a large frequency range necessary for the analysis of dynamic properties.

A key consideration of this method is the force, F(t), between the ESP and target NW which can be estimated from:

$$F(t) = \alpha \beta \left(V_{DC} + 2V_{DC} V_{AC} \cos \omega t + \frac{1}{2} V_{AC}^2 \cos 2\omega t + \frac{1}{2} V_{AC}^2 \right)$$
(1)

where α is a geometric constant, β is a proportional constant, V_{AC} and V_{DC} are the AC and DC voltage respectively, ω is the frequency of the AC voltage at the ESP and *t* is the time variable.¹ At this stage, it is important to recognise that the forcing function produces components acting at both the driving frequency (ω) and driving frequency double (2ω).

To locate the resonant frequencies of the target NWs, a frequency sweep was performed. In order to ensure that we are correctly recording the driving frequency and not its double we test at both $\times 0.5$ and $\times 2$ identified frequencies. Additionally, it is important to consider the effect of parametric

excitation which can cause resonance at a fraction of the natural frequency $(2\omega_n/i, i = 1, 2, 3...)^2$ According to earlier work from Chen *et al.*,³ parametric excitation dominates when the ESP is collinear to the sample, while forced excitation dominates when the ESP is transverse to the sample; as such we follow these recommendations to avoid parametric excitation. In tests where the resonant spectrum was desired, a frequency sweep was performed and a video micrograph was recorded. The frequencyamplitude spectrum was then extracted through our in-house image processing code.

Video micrographs of resonating nanowires

The following videos are provided as supporting information. V1 shows a NW resonating with an asymmetric resonant profile due to non-linear effects which present a large driving voltages. V2 shows a NW resonating with a typical symmetric resonant profiles.

- V1: Asymmetric resonant profile
- V2: Typical symmetric resonant profile

Comparison of damping effects and quality factor

In a nanoresonator, the main contributors to damping are thermos-elastic damping (TED), gas damping, fixture effects and surface effects.⁴ In this work, it is argued that the main contributor to damping is the surface effect, and thus the other contributors are negligible. To demonstrate this, consider an indicative GaAs NW in line with the NWs present in this work. Here a uniform cross-section NW with a length of 15 μ m, a diameter of 300 nm and a Young's modulus of 200 GPa is considered. A NW such as this will have a first mode resonant frequency of 1144 kHz.

Thermo-elastic damping

Thermo-elastic damping is caused by a coupling of the mechanical stress field and the temperature field. Zener's⁵ model says that the QF contribution due to TED is:

$$Q_{TED}^{-1} = \frac{E\alpha T_0}{C_p} \frac{\omega \tau_z}{1 + (\omega \tau_z)^2}$$
(2)

where *E* is the Young's modulus, α is the coefficient of thermal expansion, T_0 is the temperature, C_p is the heat capacity per unit volume at constant pressure, ω is the frequency, and $\tau_z = b^2/(\pi^2 \chi)$ is the relaxation time, where *b* is the beam diameter, and χ is the thermal diffusivity.

For GaAs,
$$\alpha = 6.4 \times 10^{-6} \text{ K}^{-1}$$
, $C_p = 1.78 \times 10^6 / \text{m}^{-3} / \text{K}^{-1}$ and $\chi = 2.45 \times 10^{-5} \text{ m}^2 / \text{s}^6$.

Utilising a temperature of 300 K the approximate contribution to QF from TED becomes $Q_{TED} = 2.74 \times 10^5$. As this is much larger that the QF of this measured samples, it can be concluded that the contribution due to TED.

Gas damping

Under low pressures, gas damping is caused by the momentum transfers from gas molecules colliding with the resonator – this is known as the molecular regime. The molecular regime occurs when the mean free path of the gas molecules is larger than the resonator amplitude.⁴ Under these conditions, the damping due to the surrounding gas is given by:^{4,7}

$$Q_{gas}^{-1} \approx \frac{pA}{\omega_n m_{eff} v} \tag{3}$$

where *p* is the pressure, *A* is the lateral surface area, ω_n is the resonant frequency, m_{eff} is the resonator mass, and *v* is the gas molecule thermal velocity define as $v = \sqrt{k_B T/m}$, where k_B is the Boltzmann's constant, *T* is the temperature, and *m* is the gas molecular mass.

Assuming a molecular mass of 29 g/mol, a temperature of 300 K and a pressure of 5 mPa, which was the maximum pressure during resonance, the damping due to gas is approximated at $Q_{gas} = 5.28 \times 10^8$. As the damping due to gas is much less than the measured QF, its contribution is deemed negligible.

Fixture effects

Photiadis and Judge⁸ show that for a rectangular cross-section resonator, the contribution from the fixture to QF can be approximate by:

$$Q_{fixture}^{-1} \approx 0.31 \frac{w}{l} \left(\frac{h}{l}\right)^4 \tag{4}$$

where w, h and l are the beam width, height and length respectively. While the NWs in this work are circular in cross-section, this can give an approximation of QF. Using a wost case analogy, we let w and h be equivalent to the NW diameter. From this, the contribution of Q from the fixture becomes $Q_{fixture} \approx 1.01 \times 10^9$. As the contribution of fixture effects to QF is much larger than the QF of measured samples, its contribution is negligible.

Combined effect analysis

Contributions to QF summate inversely, such that the total is given by $Q^{-1} = Q_{thermo-elastic}^{-1} + Q_{gas}^{-1} + Q_{fixture}^{-1} + Q_{surface}^{-1} + \cdots$ ⁹ In this work, QF was measured to be between 442 – 3156, which is much less than the QF of the above calculated contributors from theoretical models. Due to this, and due to the inverse summation nature of QF, these contributors can be deemed negligible and thus it is concluded that the major contributor to QF in this work is the surface effect. Furthermore, while theoretical models of surface effects are yet to be developed, the QF due to surface effects is known to be proportional to the volume to surface-area ratio.⁷ This is in line with other literature which has found

that for NW resonators, QF is dominated by surface effects, due to the high volume to surface-area ratio.¹⁰ In addition, as damping due to SFs would manifest through TED, it can be further concluded that SFs do not significantly effect QF.

Stiffness tensor comparison of zinc blende and wurtzite GaAs

In this work we characterise the core and shell Young's modulus of zinc blende (ZB) GaAs NWs, which we compare to wurtzite (WZ) GaAs NWs. To support this, we compare below the predicted Young's modulus of ZB and WZ GaAs as derived from their stiffness tensors.

Zinc Blende

Zinc blende is a cubic crystal system, as such its stiffness tensor $(C_{ZB,ij})$ is of the form:

$$\begin{bmatrix} C_{ZB,ij} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$
(2)

where the elastic constants are $C_{11} = 124.2$ GPa, $C_{12} = 51.4$ GPa, $C_{44} = 63.4$ GPa¹¹.

The directional Young's modulus (E) of a cubic system can be calculated from:¹²

$$\frac{1}{E} = S_{11} - 2\left[(S_{11} - S_{12}) - \frac{1}{2}S_{44} \right] (l_1^2 l_2^2 + l_2^2 l_3^2 + l_3^2 l_1^2)$$

where S_{ij} are the constants of the compliance tensor where the compliance tensor is the inverse of the stiffness tensor ($S_{ij} = inv(C_{ij})$), and l_1 , l_2 , and l_3 are the relevant cosines for the direction of interest.

ZB GaAs NWs grow in the [111] direction, thus the elastic modulus in the growth direction is defined by the $(l_1, l_2, l_3) = (0.577, 0.577, 0.577)$ and thus the theoretical Young's modulus of ZB GaAs NWs in the growth direction can be calculated to be 149 GPa.

Wurtzite

Wurtzite is a hexagonal crystal system, as such its stiffness tensor $(C_{WZ,ij})$ is of the form:

$$\begin{bmatrix} C_{WZ,ij} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & (C_{11} - C_{12})/2 \end{bmatrix}$$
(1)

where the elastic constants $C_{11} = 147.6$ GPa, $C_{12} = 46$ GPa, $C_{13} = 33.4$ GPa, $C_{44} = 42.2$ GPa.¹¹

WZ GaAs NWs are grown in the [001] direction, and thus their Young's modulus in the growth direction is equivalent to the Young's modulus in the z-direction of the tensor. The Young's modulus in the z-direction is defined as $1/S_{33}$, and thus the theoretical Young's modulus of WZ GaAs NWs in the growth direction can be calculated to be 149 GPa; the same as for ZB GaAs NWs.

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