Strain induced band alignment in wurtzite-zincblende InAs heterostructured nanowires

Jaya Kumar Panda and Anushree Roy
Department of Physics, Indian Institute of Technology Kharagpur 721302, India

Arup Chakraborty and Indra Dasgupta
Department of Solid State Physics,
Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700032, India

Elena Hasanu, Daniele Ercolani and Lucia Sorba
NEST-Istituto Nanoscienze-CNR and Scuola Normale Superiore,
Piazza S. Silvestro 12, I-56127 Pisa, Italy

Mauro Gemmi
Center for Nanotechnology Innovation @ NEST,
Istituto Italiano di Tecnologia, Piazza S. Silvestro 12, I-56127 Pisa, Italy

Abstract

We study band alignment in wurtzite-zincblende polytype InAs heterostructured nanowires using temperature dependent resonance Raman measurements. Nanowires having two different wurtzite fractions are investigated. Using visible excitation wavelengths in resonance Raman measurements, we probe the electronic band alignment of these semiconductor nanowires near a high symmetry point of the Brillouin zone (E₁ gap). The strain in the crystal structure, as revealed from the shift of the phonon mode, explains the observed band alignment at the wurtzite-zincblende interface. Our experimental results are further supported by electronic structure calculations for such periodic heterostructured interface.

*Electronic address: anushree@phy.iitkgp.ernet.in
†Electronic address: sspid@iacs.res.in
‡Electronic address: lucia.sorba@nano.cnr.it
I. INTRODUCTION

The electronic structure of III-V As-based semiconductors in zincblende (ZB) phase are well studied in the literature [1]. The modulation of the crystal structure in the wurtzite (WZ) phase of these semiconductors alters various physical parameters, particularly those related to their optical properties [2, 3]. More intriguing electronic band structure and related optical characteristics can be achieved by growing heterostructure of ZB and WZ phases in these systems. In the literature, the electronic band structure of WZ-ZB heterocrystalline III-V semiconductor interface has been calculated using first-principles density functional theory within local-density approximation [4, 5]. It is believed that the WZ/ZB heterostructure forms a type-II band alignment with positive valence band (VB) and conduction band (CB) offset, where the top of the valence band is defined by the WZ part while the bottom of the conduction band is hosted by the ZB portion of the heterostructure [5].

In recent years, the polytype crystal structure of III-V semiconductor nanowires (NWs) has been exploited in band gap engineering of these systems for optoelectronic device fabrication [6]. In polytype NWs, in general, one finds a periodic quantum well structure of the ZB phase as a narrow segment into the WZ phase [7]. While governing the optical characteristics of these systems, their electronic structure may not follow our understanding on the basis of a single heterostructured interface. The effect of periodicity is expected to be reflected in the band alignment, in general, and in the band offset, in particular. Heiss et. al. have demonstrated that the optical characteristics of the NWs with periodic arrangement of ZB-WZ phases along the axis are quite different from those in non-periodic interface [8].

There are quite a few report, in which the energy landscape of polytype heterostructured NWs has been explored using luminescence (photoluminescence (PL)/cathodoluminescence (CL)/time-resolved PL) measurements, thereby discuss the band alignment near the Γ point of the band structure [8–12]. These studies indicate that the optical transitions in GaAs or in InAs ZB-WZ heterostructure NWs are mostly governed by (i) band to band transitions within individual WZ and ZB phases [11–13], (ii) defect related donor-acceptor recombinations [9–11], (iii) band-acceptor transitions [10] and (iv) transition of spatially separated electrons and holes, i.e. when they are located in the different sections of ZB/WZ phases of the heterostructure [10, 13, 14]. It has been demonstrated that other factors, like the effect of ZB and WZ fractions along the axis of the wires [8, 12] and spontaneous polarization over
the valence band [10, 15], play crucial role in determining the optical transitions in such systems. The band bending due to induced space charge by spatially separated electrons and holes, typical in type II quantum well, has also been discussed in the literature [12, 16]. In polytype NWs inclusion of stacking fault/twinning in the crystal structure, the twin density and periodicity are shown to be reflected in optical transitions in these systems [8, 12, 17]. To explain the impact of such disorder in the band alignment the role of confinement of either holes or electrons in narrow segments of the NWs [8, 12] has been exploited.

Another important aspect, namely the effect of interfacial strain between ZB and WZ phases on the electronic structure of these NWs hardly received any attention. There are quite a few reports in the literature, in which the strain in the crystal of GaAs and InAs polytype NWs has been discussed [18, 19]. It is well known that the effect of strain in the crystal structure modifies the electronic band structure appreciably and cannot be ignored in a related discussion. Cheiwchanchamnangij and Lambrecht have shown the modulation of the band structure parameters with lattice strain in WZ and ZB phases of GaAs using self-consistent GW calculations [20].

Strain in a crystal structure can be modulated by temperature. As the phonon spectra are sensitive to strain in the lattice, we have carried out temperature dependent resonance Raman (RR) measurements to demonstrate the effect of strain across the WZ-ZB interface of InAs polytype NWs in modulating the band alignment. Our experimental studies are corroborated with electronic structure calculations for periodic heterostructures of WZ-ZB interface, providing further credence to the important role of strain. For visible excitation wavelengths RR spectra of InAs probe the high symmetry A point for WZ phase and L point of the ZB phase in the bulk electronic band structure. The corresponding electronic transitions at these points reflect the $E_1$ gap of these semiconductors. Here we would like to mention that the optical band gap ($E_0$ gap) of InAs in ZB and WZ phases are 0.37 eV [1] and 0.48 eV [3]. Hence, it is not possible for conventional photoluminescence measurements to probe its electronic band structure.

The remainder of the paper is organized as follows. In section II we discuss experimental and theoretical methods that we have employed in the present work. Section III is devoted to the description and discussion of our experimental and theoretical results followed by conclusions in section IV.
II. METHODOLOGY

Aligned InAs NWs were grown on InAs (111)B substrate using chemical beam epitaxy technique by employing different growth protocols in order to realize NWs with different WZ/ZB fractions (i.e. different residual strain) along the NW axis. Two different samples namely NW1 and NW2 were grown at temperatures of 400±5°C, 430±5°C, respectively and metal-organic (MO) line pressure of trimethyl indium (TMIn) of 0.3 Torr. Instead, tertiary-butyl arsine (TBAs) was varied to 0.5 Torr and 2.0 Torr for NW1 and NW2 respectively. TEM observations were carried out on a Zeiss Libra 120 transmission electron microscope operating at 120 kV and equipped with an in-column omega filter for energy filtered imaging. The NWs were transferred on a formvar carbon coated copper grid by gently rubbing the grids on the as-grown substrate.

Stokes micro-Raman measurements were carried out in back scattering geometry using a spectrometer, equipped with a microscope (model BX41 Olympus, Japan), triple-monochromator(model T64000, JY, France) and a Peltier cooled CCD detector. Several excitation lines between 476.486 nm and 568.188 nm from Ar⁺-Kr⁺ laser (Model 2018-RM, Newport, USA) were used for RR measurements. For room temperature measurements, the incident laser beam was focused on the sample using 100× (numerical aperture 0.9) objective lens and for temperature dependent measurements 50× (numerical aperture 0.5) objective lens was used. Power was kept at 100 kW/cm² to avoid the effect of laser heating. Room temperature RR spectra, reported in this article, are corrected for incident laser power, the \( \omega^4 \) law, optical properties of the material and spectral response of the experimental set up for different excitation energies \[21\]. We assumed the optical parameters of InAs in WZ phase to be the same as that of the bulk ZB phase. To carry out temperature dependent Raman measurements, a sample cell (Model THMS600, Linkam Scientific Instruments, UK) was used. We waited for at least 30 minutes to stabilize the set temperature before each measurement. To investigate the variation in band alignment with temperature, we recorded Raman spectra at different temperatures for seven different wavelengths between 476.486 nm (2.607 eV) and 568.188 nm (2.186 eV). We assumed that the optical properties of InAs do not change significantly over the temperature range of our interest \[22\]. For Raman measurements, the NWs were transferred on a Si substrate.

Electronic structure calculations were carried out in the frame-work of density functional
FIG. 1: Dark field TEM images of InAs NW segments (a) NW1 (b) NW2 recorded along the [2-1-10] WZ zone axes.

theory (DFT) as implemented in Vienna ab-initio Simulation Package (VASP) 23, 24. We have used plane wave basis set with energy cut-off of 500 eV along with projector augmented wave (PAW) method 25. Since local density approximation (LDA) and generalized gradient approximation (GGA) underestimate the band gap therefore to reproduce the experimental band gap for the bulk system, the Heyd-Scuseria-Ernzerhof (HSE06) 26, 27, hybrid functional for exchange-correlation potential with different fraction of non-local Fock exchange were used. It is observed that experimental band gap can be reproduced for the non local Fock exchange =0.18. In view of the fact that HSE calculations are computationally expensive, generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional 28 was used for the electronic structure calculations of NW heterostructure with large number of atoms in the unit cell.

III. RESULTS AND DISCUSSION

A. Polytypism in NWs/Crystal structure of NWs

The crystal structure of InAs NWs with different WZ/ZB fractions has been characterized by dark field transmission electron microscope (DFTEM) images taken along [2-1-10] WZ (parallel to [110] ZB) zone axis. In this orientation, ZB and WZ crystal structures show two different diffraction patterns in which the spots belonging to one phase are well separated from those of the other. Therefore, a DFTEM image, obtained by selecting the spots of one of the two phases, gives a contrast in which stacking faults and polytype changes can be
FIG. 2: Non-resonant Raman spectra recorded at 100K for (a) bulk, (b) NW1 (99% WZ), and (c) NW2 (80% WZ). Experimental data points are shown by + symbols and the net fitted spectra by solid lines. The deconvoluted phonon modes are shown by dashed lines.

easily identified. Characteristic DFTEM images of two different NWs designated as NW1 and NW2 are shown in Fig. 1. The average fraction of WZ phase, estimated by analyzing DFTEM images of at least 20 NWs for each sample, are (99±1)% and (80±4)% for NW1 and NW2, respectively. The diameters of NW1 and NW2 are 31±2 nm and 56±3 nm, respectively. The corresponding lengths are 2.0±0.2 µm and 2.5±0.2 µm.

Fig. 2 shows non-resonant Raman spectra of bulk InAs in ZB phase and NW1, recorded at 100K using 496.507 nm as the excitation wavelength. To assign the phonon modes, we deconvoluted each spectrum with Lorentzian functions, keeping the Raman shift, width and intensity of all phonon modes as free fitting parameters. The deconvoluted components are shown by dashed lines in Fig. 2. For bulk InAs in ZB phase the TO and LO phonon modes appear at 217 cm⁻¹ and 239 cm⁻¹, respectively [29]. For NW1 in predominantly WZ phase, an additional \( E_{2}^{H} \) mode at 213 cm⁻¹ appears in the spectrum due to L-point folding of the Brillouin zone of the ZB phase in the modified crystal structure [18, 30]. In Fig. 2(c), the non-resonant spectrum for NW2 with 80% WZ fraction is found to be very similar to that obtained for NW1.
FIG. 3: Evolution of Raman shift of the TO phonon mode with temperature for NW1 and NW2.

B. Observation of strain in the crystal structure of NWs

The strain in a crystal structure is reflected in phonon wavenumber. Fig. 3 compares the variation of the Raman shift of the TO phonon mode ($\omega_{TO}$), over the temperature range between 120K and 300K for NW1 and NW2. Due to the increase in anharmonicity in the crystal structure, one expects a decrease in $\omega_{TO}$ with temperature [31], as observed in Fig. 3. However, we find that the value of the phonon frequency is appreciably higher in case of NW2 than in NW1. It is reasonable to assume that the crystal structure of NW1, with 99% WZ phase, is nearly strain free. Hence, we attribute the observed higher values of $\omega_{TO}$, obtained for NW2 (in comparison with NW1, see Fig. 3), to be due to the net compressive strain in its crystal structure. It is to be recalled (refer to Fig. 1) that in NW2 there are large number of ZB segments within the WZ segments of the NW. There is an appreciable difference in lattice parameters between the two phases of InAs [33] (also refer to the next section) that may aid in producing strain in NW2. We believe that the interfacial strain between two phases results in a higher Raman shift in NW2 than in NW1. On the basis of our assumption that the crystal structure of NW1 with 99% WZ fraction is nearly strain free, the above discussion implies the existence of strain in the crystal structure of NW2,
FIG. 4: Calculated electronic energy band diagram near \( E_1 \) gap at 0K of (a) ZB-InAs and (b) WZ-InAs, as obtained from DFT calculations using hybrid functionals. The high symmetry points, discussed in this article, are marked by blue dashed lines.

with 80% WZ fraction. Therefore, the effect of strain on the physical properties related to the crystal structure of these NWs cannot be ignored.

C. Bulk electronic band structure of InAs

Next we calculate electronic band structures of InAs in both ZB and WZ phases, using hybrid functional method as implemented in density functional theory (DFT). Fig. 4 (a) and (b) present the calculated band structures in these two phases. In our calculation, we used the lattice parameter \( a = 6.040 \, \text{Å} \) for the ZB phase \[34\]. We estimate the fundamental band gap for ZB-InAs at 0K to be 0.378 eV. The \( E_1 \) gap (band gap near the L point of the Brillouin zone) has been evaluated as 2.568 eV. The lattice parameters for WZ structure are obtained from that of the ZB structure using the relation

\[
a_{\text{WZ}} = \frac{a_{\text{ZB}}}{\sqrt{2}}\]  

(1)
FIG. 5: Band alignment at high symmetry point at WZ-ZB heterointerface (as obtained from the green marked regions in 4 (a) and (b)). All possible transition energies (in eV) are also marked. The solid arrows indicate band to band transitions and the dashed arrow corresponds to transition of spatially separated carriers.

\[ c_{WZ} = \sqrt[3]{\frac{8}{3}} a_{WZ} \]  

The estimated lattice parameters for the WZ phase are \( a=4.2709 \) Å and \( c=6.9744 \) Å. For the WZ phase, the \( E_1 \) gap (A point of the Brillouin zone) at 0K is estimated to be 2.432 eV. We find the difference in calculated \( E_1 \) gap-energies of two phases to be \( \sim 136 \) meV.

In order to obtain the \( E_1 \) band alignment at the ZB-WZ heterointerface near the high symmetry point (corresponding to L and A points of the Brillouin zone of ZB and WZ phases respectively), we consider the portion of the band structure marked by blue dashed lines in Fig. 4(a) and 4(b). The schematic band alignment near WZ-ZB heterointerface, thus obtained, is shown in Fig. 5 and is of type-II, where the valence band maximum and conduction band minimum are located in WZ and ZB region respectively. This alignment of the \( E_1 \) gap is very similar to that obtained for the \( E_0 \) gap for a ZB-WZ interface. As mentioned earlier, in the absence of any defect related states in type II band alignment of a quantum well one expects either localized band to band electronic transitions in the well and in the barrier regions (blue arrows in Fig. 5), or transition forming spatially separated
holes and electrons (orange arrow). The corresponding calculated transition energies from the bulk band structure are 2.568 eV, 2.432 eV and 2.890 eV, respectively.

D. Electronic structure as obtained from resonance Raman measurements

Light does not interact directly with phonons in a crystal. The incident photon excites the electron from its ground state and creates an electron-hole pair. This electron or hole interacts with a phonon and creates a new excited state. Next, the electron and hole recombines and we get the scattered photon. When the value of the excitation energy coincides with that of the electronic band gap, resonance occurs. Thus, RR measurements probe the electronic band structure of semiconductors. Raman spectroscopy exploits the coupling of different phonon modes with the electronic states, following the selection rules. Governed by Raman selection rules, RR scattering reveals symmetries of the electronic states.

We have carried out RR measurements to probe the band alignment in NWs. For comparison, we also study RR spectra of bulk InAs, in the usual ZB phase. For RR measurement, Raman spectra of bulk InAs and NWs are recorded at different excitation energies (over the range between 2.340 and 2.607 eV). It is to be noted that the given range of excitation energies covers a wide range of the visible spectrum (530 nm to 568 nm) and RR scattering occurs, coupling the energy states of the E₁ gap of InAs. Fig. 6(a)-6(c) present the variation in intensity of the strong TO phonon mode for bulk and NWs for different excitation energies. The resonance energies at 2.56±0.02 eV, 2.46±0.02 eV and 2.55±0.02 eV are observed for bulk, NW1 and NW2, respectively. For NW1 with 99% WZ fraction the resonance energy is 110 meV less than that of bulk InAs of ZB phase, which is close to the calculated (136 meV) difference in the E₁ gap of ZB and WZ structure of InAs. These values match the earlier report [35] on difference in E₁ gap of InAs in ZB and WZ phases fairly well. Interestingly, for NW2 with 80% WZ fraction, the resonance energy is observed to be 2.55 eV, a value close to that of InAs in the ZB phase.

Keeping in mind that interfacial strain can modify the band alignment and to explain the observed difference in resonance energy in NW1 and NW2, we propose a possible explanation for the observed resonance energy of NWs and hence, plausible band alignment at the heterointerface. For nearly strain-free NW1 with 99% WZ fraction, Raman resonance occurs
FIG. 6: Variation in intensity of the TO phonon mode at room temperature for different excitation energies (a) bulk InAs, (b) NW1 and (c) NW2.

at 2.46 eV due to minimum energy band to band transitions at the WZ segment of the wire (see Fig. 5). The band gap in the ZB segment remains at 2.56 eV (as observed in bulk ZB-InAs). As the ZB fraction in this set of wires is only 1%, the phonon creation is dominated by band to band transition of electrons in the WZ segment. The spatially separated transition (ZB→WZ) could not be observed, since the corresponding energy is beyond the range of excitation energies used by us.

To anticipate the possible band alignment in NW2, we refer to Fig. 3, where we have plotted the variation of $\omega_{TO}$ with temperature. We attributed the observed differences in the phonon characteristic of NW1 and NW2 to be a consequence of compressive strain in the crystal structure of the latter. For resonance energy of NW2 to be the same as that of InAs of ZB phase, one of the possibilities is a lowering of both valence and conduction band edge of the WZ phase, so that they match with those of the ZB phase. The proposed band alignment in NW2 is shown in Fig. 7. It is to be noted that for strain-induced shift in the
conduction or valence band edge of the ZB segment the resonance would have occurred at
different excitation energies, not exactly at 2.55 eV, which corresponds to a gap of the ZB
phase. Further, if the conduction (valence) band edge of the WZ phase lies below (above)
the one we show schematically in Fig. 7, then the energy gap of the WZ phase will be less
than the lowest probing excitation energy, used by us. In that case, the observed resonance
is still expected to be governed by the band to band transition of the ZB phase.

E. Theoretical justification for strain induced band alignment

In order to understand the band alignment due to ZB-WZ interface in NW2, we con-
structed a model of coupled WZ-ZB NW from bulk supercell structure that closely resemble
the crystal structure of NW2. In the model structure, the WZ NW consists of 72 In and 72
As atoms and ZB NW consists of 31 In and 31 As atoms. As a consequence the diameter
of both the systems are 1.4 nm while their lengths are 1.82 nm and 0.77 nm respectively.
The dangling bonds at the surface of the NWs are saturated by pseudo hydrogen atoms
[36]. The concentration of the ZB part in this model NW heterostructure is 30%. The (111)
As terminated polar facet of ZB is attached to the (0001) polar facet of WZ containing In
atoms. We have considered the system to be periodic (-ZB-WZ-ZB-) along its length. In

FIG. 7: Expected band alignment at heterointerface of NW2.
FIG. 8: (a) Density of states (DOS) for the periodic ZB-WZ coupled NW with 30% ZB part; (b) Iso-surface (in green color) of charge density for VBM and CBM of the periodic coupled NWs (30% ZB); In(WZ), As(WZ), In(ZB), As(ZB), H atoms are in grey, blue, magenta, yellow, and, sky blue color respectively. (c) energy resolved charge density plot for the periodic coupled NWs with 30% ZB part. (d) strain profile across the interface for the coupled ZB-WZ periodic NWs.

order to reduce the cost of computation, although the calculations are done for 30% ZB, our results are expected also to hold good for 20% ZB NWs realized experimentally.

The density of states (DOS) for the periodic coupled NW (see Fig. 8(a)) reveal that the gap between valence band maximum (VBM) and the conduction band minimum (CBM) to be 1.15 eV. Interestingly the band gap for a WZ NW (diameter = 1.4 nm) is 1.18 eV while that for ZB NW of same diameter is calculated to be 1.14 eV, suggesting that the band gap for the coupled ZB-WZ periodic NW is very close to that obtained for the ZB system. As mentioned earlier (Section IIIc), this band alignment for the $E_0$ gap is also expected to hold good for the $E_1$ gap. Our calculations of the charge density (see Fig. 8(b)) and energy resolved charge density (see Fig. 8(c)) further reveal that for the periodic system there is no band offset at the interface. The plot of the charge density for the valence band maximum (VBM) and the conduction band minimum (CBM)(see Fig. 8(b)) show that the charge density is delocalized and spread both in the ZB and WZ part of the coupled NW.
The energy resolved charge density plot shown in Fig. 8(c) clearly reveal the absence of band offset both in the valence band and the conduction band. Finally we have calculated the strain profile for the coupled quantum NW following the method proposed in ref. [37] where the trace of the strain tensor that represents the volumetric strain is calculated for the system. The results of our calculation for the cationic and anionic planes are displayed in Fig. 8(d). The strain in the anion plane is tensile while the strain in the cation plane is compressive. In contrast to coupled quantum dots [37], we not only find appreciable strain at the interface but also substantial strain even far away from the interface. The strain profile is nearly constant for the anion plane but oscillating for the cation plane. Such large value of strain is expected to have profound impact on the band alignment as anticipated from the experimental results discussed in the previous section.

**F. Temperature variation of the band alignment**

![Graph showing the intensity of the TO phonon mode at different temperatures for different excitation energies](image)

**FIG. 9:** Intensity of the TO phonon mode at different temperatures for different excitation energies (a) bulk InAs, (b) NW1 and (c) NW2. The solid lines are guide to the eyes.

The strain in a crystal is sensitive to the temperature. We have probed the change in the band gaps of NW1 and NW2 with temperature. We recorded Raman spectra of both bulk and NWs at different temperatures for various excitation energies. The spectra are recorded
FIG. 10: Variation in resonance energy with temperature of bulk, NW1 and NW2. The calculated (scaled) variation of the $E_{1}$ gap with temperature for WZ and ZB phases are shown by blue solid line and green dashed line, respectively.

at different temperature range between 120K and 750K for each excitation wavelength. The intensity of the TO phonon mode for each spectrum was estimated. The data points in Fig. 9 (a), (b) and (c) correspond to the integral intensity of the TO phonon mode at the given temperature for bulk-InAs, NW1 and NW2, respectively. The dashed lines indicate the shift in temperature at which resonances were obtained at different excitation energies. In Fig. 10 we present the variation of the resonance energy with temperature for bulk InAs and NWs, as obtained from Fig. 9 (plots the maximum of the temperature-response curve in each panel in Fig. 9 (a), (b) and (c)). It is to be recalled that by RR measurements we probe the $E_{1}$ gap of InAs and thus, the above measurements reveal the temperature variation of the high symmetry point in the band structures of the bulk and the NW systems.

We have calculated the variation of the $E_{1}$ gap for the WZ and the ZB with temperature. For the ZB phase, the values of the lattice parameter at different temperatures are obtained from Ref. [34]. Due to unavailability of the lattice parameters of WZ-InAs at different temperatures, we calculated the temperature dependent lattice parameters for the WZ phase
using $a_{ZB}$ and the relations described in Eqn.1 and Eqn.2. The variation in $E_1$ gap of ZB and WZ phases with temperature, as obtained from the DFT+hybrid calculations, are shown in Fig. 10 by green (dashed) and blue (solid) lines, respectively. The theoretically estimated $E_1$ vs T plot are scaled to match with the experimental data points. We find that though the variation of the resonance energy with temperature in NW1 is like one expects for the WZ phase, the same for NW2 is similar to that of the ZB phase. Thus, we independently confirm the dominating ZB-like behavior of the band alignment in NW2 for a wide range of temperature from 120K to 750K under visible light.

IV. CONCLUSION

In this article we correlate the band alignment in InAs WZ-ZB heterostructured NWs with different WZ fractions, with the lattice strain in their crystal structure. While RR measurements probed the high symmetry points of the electronic band structure of InAs, the strain in the crystal structure is revealed from the shift of the phonon modes. Theoretical simulation on model system confirm the dominating ZB like behavior for the band alignment for NW2 with 20% ZB fraction. We have demonstrated the ZB-like behavior of the band alignment in InAs WZ-ZB polytype NWs with 20% ZB fraction, over a wide temperature range.

V. ACKNOWLEDGEMENT

ID thanks DST India and Cray Super Computer facility in IACS Kolkata.

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