I. INTRODUCTION

Silicon nanowires (SiNW) can be well produced in different directions with different diameters.[1–6] It is a promising candidate for nano-device, and has attracted a lot of interest.[7–19] The SiNW can serve as basic building blocks for electrically based sensor[7–10], field effect transistor[11–16] and logic gates[17], photovoltaic device[18], and functional networks[19]. The possible stable configurations of the SiNW have been investigated with density-functional tight-binding simulations by Zhang *et al.* in Refs. 20. They found that the stability of SiNW is determined by the competition between the minimization of the surface energy and the minimization of the surface-to-volume ratio. As one of the important thermal properties in SiNW, the thermal expansion plays an important role for these applications in the electronic or thermal devices. The thermal expansion effect can be studied in the classical molecular dynamics.[21]

In this paper, we first analyze various phonon vibrational modes in SiNW from the Tersoff potential[22] implemented in the "General Utility Lattice Program" (GULP).[23] Some important features of phonon modes in SiNW of different directions and with different structure ratio $\gamma = length/diameter$ are discussed. We then investigate the coefficient of thermal expansion (CTE) of SiNW in [100], [110] and [111] growth directions by the nonequilibrium Green's function approach[24], which is a quantum mechanical method and automatically includes contribution of all phonon modes. We find that at low temperatures, all SiNW studied have thermal contraction effect and the CTE in SiNW [110] is the largest one among the three directions. The CTE decreases rapidly with increasing structure ratio γ, and is negative in whole temperature range with $\gamma = 1.3$.

II. RESULTS AND DISCUSSION

Fig. 1 demonstrates that a SiNW with length and diameter (L, D) can be cut from the bulk Si crystal by using a virtual cylinder with structure parameters (L, D).[25] We can cut SiNW in different growth directions: [100], [110] and [111], by controlling the direction of the virtual cylinder. The SiNW displayed in the figure is in [100] growth direction with (L, D)=(3, 1) nm. As discussed in Refs. 26, it is not important to include H-passivation on the surface for thermal property of SiNW. We adopt this approximation which may introduce