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Analysis of single- and double-barrier tunneling diode structures using ultra-thin-CaF_2/CdF_2/Si multilayered heterostructures grown on Si

Keita Suda, Yuya Kuwata and Masahiro Watanabe

Department of Electronics and Applied Physics
Interdisciplinary Graduate School and Engineering, Tokyo Institute of Technology.
4259-J2-71, Nagatsuta-cho, Midori-ku, Yokohama-shi, Kanagawa 226-8502, Japan
Phone: +81-45-924-5454 E-mail: suda.k.ae@m.titech.ac.jp

Abstract:

Current-voltage characteristics of the single-barrier and double-barrier tunneling diodes using Si/CaF_2/CdF_2 ultra-thin layered heterostructures grown on Si substrates have been theoretically analyzed and evaluated material parameters such as conduction band discontinuity (ΔE_C) at the heterointerface and effective masses via fitting with experimental I-V characteristics. It has been found that the ΔE_C between a few monolayer of CaF_2 and Si was estimated as 1.5-1.7 eV, which was 30% smaller than the reported value for the bulk CaF_2. The estimated values are consistent with the negative differential resistance characteristics for the double-barrier resonant tunneling diode structures.

1. Introduction

The dimension of the elements consisting integrated circuits is going down into nano-scale. One essential building block for nanoscale solid state devices is electric potential sequences for controlling electron transport, which can be implemented using energy band discontinuity at atomically abrupt heterointerfaces. A CdF_2/CaF_2/Si heterostructure is an attractive candidate for applications on Si substrates, such as resonant tunneling diodes (RTDs) [1] and transistors [2], resistance switching devices [3,4], because of the large conduction band discontinuity (ΔE_C~2.3eV) at the heterointerface [5,6] and small lattice mismatch with silicon. To date, we have demonstrated large ON/OFF current ratio of CdF_2/CaF_2 RTDs larger than 10^5 at room temperature (RT) [1,7,8], which confirmed advantage of the large ΔE_C heterostructure material systems. In order to establish the design paradigm of the tunneling devices using heterostructure materials, the modeling of electron transport and key material parameters such as conduction band discontinuity and effective masses for atomically-thin layers are essentially important for design and optimization of the device performance. Recent results of our study strongly suggest that some material parameters such as the barrier height of a few monolayer of CaF_2 is smaller than that for the "thick" CaF_2 layer, which would strongly affect tunneling current density. In this study, we have carried out systematic fitting simulation of I-V curve for the structure of single-barrier and double-barrier tunneling diode focusing on parameters of ΔE_C and effective mass of CaF_2.

2. Calculation method and sample preparation

Tunneling current was calculated using transfer-matrix method and Esaki-Tsu formula [9,10] based on the effective mass approximation and self-consistent potential scheme. The effect of the voltage drop due to accumulation and depletion of carriers in Si layer was considered in the calculation. In this study, I-V curves of Al/CaF_2/Si single-barrier and Si/CaF_2/CdF_2/CaF_2/Si double-barrier tunneling diode structures with a few monolayer-thick-CaF_2 barrier layers were investigated theoretically and experimentally. In the calculation, material parameters such as the effective mass of CaF_2 (m*) and the band discontinuity between Si and CaF_2 (ΔE_C) were varied in the range of m* = 0.1-1.0 m_0 and ΔE_C=0.5-2.3 eV, respectively, where m_0 indicates the free electron mass. Samples for I-V measurement were grown on Si(111) substrates using the growth method based on the MBE technique reported in ref.[4]. Diameter of the contact window was 2.2 μm and Au/Al contact electrode was formed by lift-off.

3. Results and Discussion

Figure 1 shows I-V characteristics of single-barrier tunneling diode with the CaF_2 barrier layer with the thickness of (a) 0.93 nm and (b) 1.55 nm, where the schematic conduction band profile is shown in the inset. The circle and rectangular points are measurement results at RT. The solid line and the dashed line are calculated results fitted using the parameters of (a) m*=1.0m_0 and ΔE_C=1.5eV and (b) m*=0.7m_0 and ΔE_C=1.7eV, respectively. Measured I-V curves were well reproduced by the fitting simulation, as shown in the figure. The values of ΔE_C estimated as in the range of 1.5-1.7eV are 26-35% smaller than the value for the reported bulk CaF_2-Si heterointerface (ΔE_C~2.3eV) [5,6], which would suggest the deviation due to the atomically-thin layer thickness of CaF_2.

Figure 2 shows one example of experimental I-V characteristics at RT of Si(4.96nm)/CaF_2(0.93nm)/ CdF_2(2.48 nm)/CaF_2(0.93nm)/i-Si(0.93nm)/Al double-barrier resonant-tunneling quantum-well structure reported in ref.[4], where the conduction band profile of the device structure is schematically shown in Fig. 3. Peak current density and peak voltage of the negative differential resistance characteristics were calculated and plotted in Fig. 4 as a parameter of m^*_{CaF2} = 0.1-1.0 m_0 and ΔE_C between Si-CaF_2 = 0.5-2.3 eV, where the effective mass of CdF_2 quantum-well layer = 0.40m_0, the band discontinuity between Si and CdF_2 =

-0.6[eV]. A solid star indicates one example of experimental results shown in Fig. 2. It was found that the experimental data locates near the calculated points of m* ≈0.7m_0 and ΔE_C=1.7eV, which is consistent with the result of Fig. 1. Actually, the effective mass of CdF_2 and conduction band discontinuity between CaF_2 and CdF_2 are also important parameter especially for peak voltage. Detail of the fitting simulation including these parameters will be also discussed.

4. Conclusion

Current-voltage characteristics of the atomically-thin single- and double-barrier tunneling diode structures were theoretically analyzed and fitted with measurement results for precise evaluation of material parameters such as ΔE_C and m*. It was found that conduction band discontinuity of Si/CaF_2 heterointerface would be around 30% smaller than the reported value of bulk CaF_2 layers.

References

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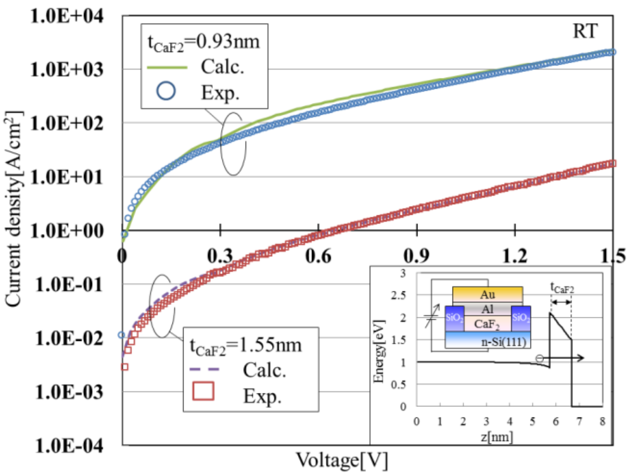

Fig. 1 Theoretical and experimental I-V characteristics of CaF_2 single-barrier tunneling diode with the barrier layer thickness of (a) 0.93nm, (b) 1.55nm. Inset shows the band diagram of the structure at applied voltage of 1V.

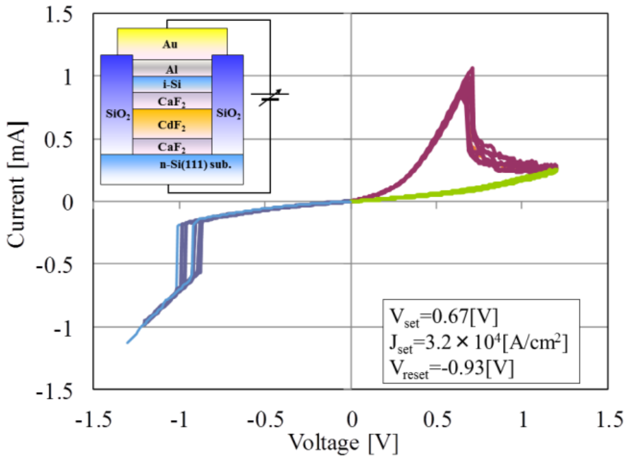

Fig. 2 I-V characteristics measured at room temperature of n-Si/CaF_2(0.93nm)/CdF_2(2.48nm)/CaF_2(0.93nm)/ i-Si(0.93nm)/Al double-barrier structure[4].

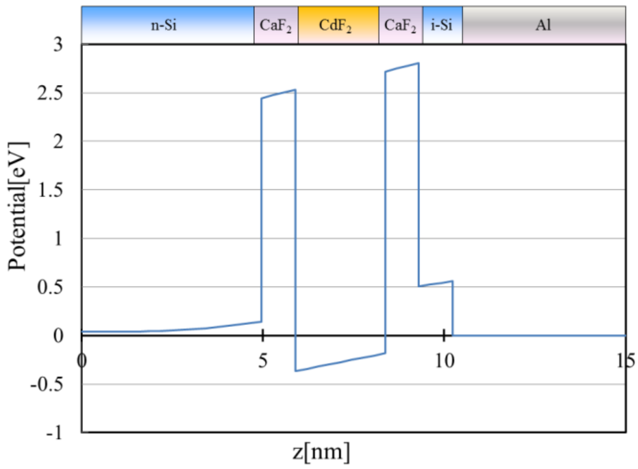

Fig. 3 An analysis model of conduction band profile of double-barrier resonant tunneling diode structure.

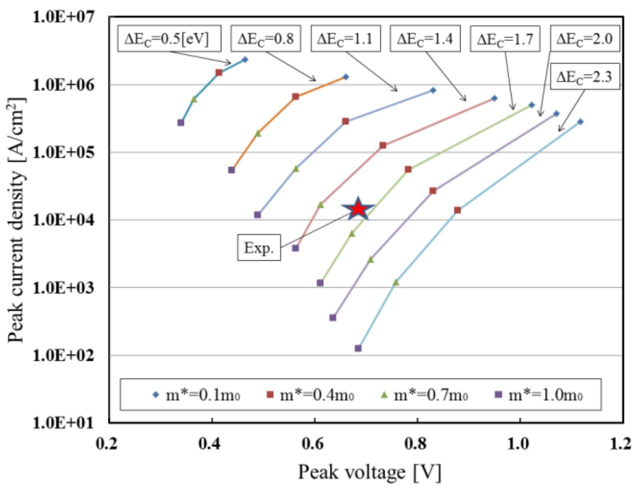

Fig. 4 Peak voltage vs peak current density of negative differential characteristics of double-barrier tunneling structures as parameters of m* of CaF_2 and ΔE_C.