

多势垒结构共振透射系数的计算

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[摘要] 使用转移矩阵方法精确求解了一维定态薛定谔方程,求出了在多势垒结构中电子能量大于、等于、小于势垒高度情况下的共振透射系数的表达式,并进一步研究了多势垒结构的共振透射系数与有效质量和势垒宽度及势垒个数之间的关系.

[关键词] 转移矩阵,共振透射系数,多势垒结构

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Calculation of Resonant Transmission Coefficient for Multi-Barrier Structure

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Abstract: The resonant transmission coefficient of multi-barrier structure is presented based on an exact solution of the Schrödinger equation by using the transfer matrix approach under the case of the incident electron energy being greater than , equal to , and less than the barrier height; furthermore , we have also studied the relationship between the resonant transmission coefficient and the effective mass , the barrier width , and the number of barriers.

Key words: transfer matrix method , resonant transmission , multi-barrier structure

自从超晶格的概念^[1]被提出来,同时由于分子束外延(MBE)、金属氧化物沉积(MOCVD)^[2]等制备超晶格技术的不断完善,超晶格被越来越多地研究^[3-7].超晶格是一种由两种材料交替生长而成具有周期性的半导体结构,窄带隙的材料构成势阱,宽带隙的材料构成势垒^[8].本文通过多势垒结构计算了透射系数及其与多势垒结构各参数之间的关系.

1 模型与理论

本文采用的多势垒结构如图 1 所示,其中 N 为势垒的个数, v_0 为势垒高度,势垒和势阱中电子的有效质量分别为 m_b^* 和 m_w^* ,势垒和势阱宽度分别为 a 、 b .

在势垒和势阱区中直接求解一维薛定谔方程:

(1) $E > v_0$

在 1 区: $\psi_1 = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$,

在 2 区: $\psi_2 = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}$,

在 3 区: $\psi_3 = A_3 e^{ik_3 x} + B_3 e^{-ik_3 x}$,

在 4 区: $\psi_4 = A_4 e^{ik_4 x} + B_4 e^{-ik_4 x}$,

⋮

在 $2N$ 区: $\psi_{2N} = A_{2N} e^{ik_{2N} x} + B_{2N} e^{-ik_{2N} x}$,

在 $2N+1$ 区: $\psi_{2N+1} = A_{2N+1} e^{ik_{2N+1} x} + B_{2N+1} e^{-ik_{2N+1} x}$,

其中:

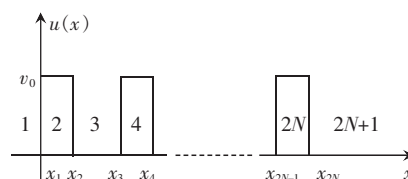


图 1 一维多势垒结构

Fig.1 One dimensional multi-barrier structure

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$N \rightarrow$ 为势垒的个数

$$k_1 = k_3 = \cdots = k_{2N-1} = k_{2N+1} = \sqrt{\frac{2m_j^* E}{\hbar^2}}, j = 1, 3, \cdots, 2N-1, 2N+1, m_1^* = m_3^* = \cdots = m_{2N-1}^* = m_{2N+1}^*$$

$$k_2 = k_4 = \cdots = k_{2N-2} = k_{2N} = \sqrt{\frac{2m_j^* (E - v_0)}{\hbar^2}}, j = 2, 4, \cdots, 2N-2, 2N, m_2^* = m_4^* = \cdots = m_{2N-2}^* = m_{2N}^*$$

由在边界点 $x_1, x_2, x_3, x_4, \cdots, x_{2N-1}, x_{2N}$ 处波函数及其一阶导数连续 ($\psi_j = \psi_{j+1}, \frac{1}{m_j} \psi_j' = \frac{1}{m_{j+1}} \psi_{j+1}'$) 并由转移矩阵计算可得:

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} e^{ik_1 x_1} & 0 \\ 0 & e^{-ik_1 x_1} \end{pmatrix}^{-1} \times \begin{pmatrix} 1 & 1 \\ i \frac{k_1}{m_1^*} & -i \frac{k_1}{m_1^*} \end{pmatrix}^{-1} \times M_2 \times M_3 \times \cdots \times M_{2N-1} \times M_{2N} \times \begin{pmatrix} 1 & 1 \\ i \frac{k_{2N+1}}{m_{2N+1}^*} & -i \frac{k_{2N+1}}{m_{2N+1}^*} \end{pmatrix} \times \begin{pmatrix} e^{ik_{2N+1} x_{2N+1}} & 0 \\ 0 & e^{-ik_{2N+1} x_{2N+1}} \end{pmatrix} \times \begin{pmatrix} A_{2N+1} \\ B_{2N+1} \end{pmatrix},$$

其中:

$$\begin{aligned} M_2 &= \begin{pmatrix} \cos[k_2(x_2 - x_1)] & -\frac{1}{k_2^*} \sin[k_2(x_2 - x_1)] \\ \frac{k_2}{m_2^*} \sin[k_2(x_2 - x_1)] & \cos[k_2(x_2 - x_1)] \end{pmatrix}, \\ M_3 &= \begin{pmatrix} \cos[k_3(x_3 - x_2)] & -\frac{1}{k_3^*} \sin[k_3(x_3 - x_2)] \\ \frac{k_3}{m_3^*} \sin[k_3(x_3 - x_2)] & \cos[k_3(x_3 - x_2)] \end{pmatrix}, \\ &\vdots \\ M_{2N-1} &= \begin{pmatrix} \cos[k_{2N-1}(x_{2N-1} - x_{2N-2})] & -\frac{1}{k_{2N-1}^*} \sin[k_{2N-1}(x_{2N-1} - x_{2N-2})] \\ \frac{k_{2N-1}}{m_{2N-1}^*} \sin[k_{2N-1}(x_{2N-1} - x_{2N-2})] & \cos[k_{2N-1}(x_{2N-1} - x_{2N-2})] \end{pmatrix}, \\ M_{2N} &= \begin{pmatrix} \cos[k_{2N}(x_{2N} - x_{2N-1})] & -\frac{1}{k_{2N}^*} \sin[k_{2N}(x_{2N} - x_{2N-1})] \\ \frac{k_{2N}}{m_{2N}^*} \sin[k_{2N}(x_{2N} - x_{2N-1})] & \cos[k_{2N}(x_{2N} - x_{2N-1})] \end{pmatrix}, \end{aligned}$$

令 $M = M_2 \times M_3 \times \cdots \times M_{2N-1} \times M_{2N} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$ 则

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} e^{ik_1 x_1} & 0 \\ 0 & e^{-ik_1 x_1} \end{pmatrix}^{-1} \times \begin{pmatrix} 1 & 1 \\ i \frac{k_1}{m_1^*} & -i \frac{k_1}{m_1^*} \end{pmatrix}^{-1} \times \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \times$$

$$\begin{pmatrix} 1 & 1 \\ i \frac{k_{2N+1}^*}{m_{2N+1}^*} & -i \frac{k_{2N+1}^*}{m_{2N+1}^*} \end{pmatrix} \times \begin{pmatrix} e^{ik_{2N+1}x_{2N+1}} & 0 \\ 0 & e^{-ik_{2N+1}x_{2N+1}} \end{pmatrix} \times \begin{pmatrix} A_{2N+1} \\ B_{2N+1} \end{pmatrix},$$

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \frac{1}{2} \times \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \times \begin{pmatrix} A_{2N+1} \\ B_{2N+1} \end{pmatrix},$$

其中:

$$S_{11} = \left[\left(H_{11} + \frac{H_{21}}{i \frac{k_1^*}{m_1^*}} \right) + i \frac{k_{2N+1}^*}{m_{2N+1}^*} \left(H_{12} + \frac{H_{22}}{i \frac{k_1^*}{m_1^*}} \right) \right] e^{-ik_1x_1} e^{ik_{2N+1}x_{2N+1}},$$

$$S_{12} = \left[\left(H_{11} + \frac{H_{21}}{i \frac{k_1^*}{m_1^*}} \right) - i \frac{k_{2N+1}^*}{m_{2N+1}^*} \left(H_{12} + \frac{H_{22}}{i \frac{k_1^*}{m_1^*}} \right) \right] e^{-ik_1x_1} e^{-ik_{2N+1}x_{2N+1}},$$

$$S_{21} = \left[\left(H_{11} - \frac{H_{21}}{i \frac{k_1^*}{m_1^*}} \right) + i \frac{k_{2N+1}^*}{m_{2N+1}^*} \left(H_{12} - \frac{H_{22}}{i \frac{k_1^*}{m_1^*}} \right) \right] e^{ik_1x_1} e^{ik_{2N+1}x_{2N+1}},$$

$$S_{22} = \left[\left(H_{11} - \frac{H_{21}}{i \frac{k_1^*}{m_1^*}} \right) - i \frac{k_{2N+1}^*}{m_{2N+1}^*} \left(H_{12} - \frac{H_{22}}{i \frac{k_1^*}{m_1^*}} \right) \right] e^{ik_1x_1} e^{-ik_{2N+1}x_{2N+1}}.$$

现在我们假定具有一定能量的粒子由多势垒结构的最左边 ($x < 0$) 向右方入射, 则在1区有入射波和反射波, 在 $2N+1$ 区中由于没有由右向左运动的粒子, 因此只有透射波 ($A_{2N+1} \neq 0$), 没有向左传播的波 ($B_{2N+1} = 0$). 根据透射系数的定义^[10] 可得:

$$T = \frac{J_T}{J} = \frac{\frac{k_{2N+1}^*}{m_{2N+1}^*}}{\frac{k_1^*}{m_1^*}} \left| \frac{A_{2N+1}}{A_1} \right|^2.$$

由 $k_{2N+1} = k_1$, $m_1^* = m_{2N+1}^*$ 得:

$$T = \frac{4}{H_{11}^2 + \left(\frac{k_{2N+1}^*}{m_{2N+1}^*} H_{12} \right)^2 + \left(\frac{1}{\frac{k_1^*}{m_1^*}} H_{21} \right)^2 + H_{22}^2 + 2H_{11}H_{22} - 2H_{12}H_{21}}.$$

(2) $E = v_0$

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} e^{ik_1x_1} & 0 \\ 0 & e^{-ik_1x_1} \end{pmatrix}^{-1} \times \begin{pmatrix} 1 & 1 \\ i \frac{k_1^*}{m_1^*} & -i \frac{k_1^*}{m_1^*} \end{pmatrix}^{-1} \times M_2 \times M_3 \times \cdots \times M_{2N-1} \times M_{2N} \times$$

$$\begin{pmatrix} 1 & 1 \\ i \frac{k_{2N+1}^*}{m_{2N+1}^*} & -i \frac{k_{2N+1}^*}{m_{2N+1}^*} \end{pmatrix} \times \begin{pmatrix} e^{ik_{2N+1}x_{2N+1}} & 0 \\ 0 & e^{-ik_{2N+1}x_{2N+1}} \end{pmatrix} \times \begin{pmatrix} A_{2N+1} \\ B_{2N+1} \end{pmatrix},$$

其中:

$$M_2 = \begin{pmatrix} 1 & -m_2^* (x_2 - x_1) \\ 0 & 1 \end{pmatrix},$$

$$M_3 = \begin{pmatrix} \cos[k_3(x_3 - x_2)] & -\frac{1}{\frac{k_3^*}{m_3^*}} \sin[k_3(x_3 - x_2)] \\ \frac{k_3^*}{m_3^*} \sin[k_3(x_3 - x_2)] & \cos[k_3(x_3 - x_2)] \end{pmatrix},$$

$$\vdots$$

$$\mathbf{M}_{2N-1} = \begin{pmatrix} \cos[k_{2N-1}(x_{2N-1} - x_{2N-2})] & -\frac{1}{\frac{k_{2N-1}^*}{m_{2N-1}^*}} \sin[k_{2N-1}(x_{2N-1} - x_{2N-2})] \\ \frac{k_{2N-1}^*}{m_{2N-1}^*} \sin[k_{2N-1}(x_{2N-1} - x_{2N-2})] & \cos[k_{2N-1}(x_{2N-1} - x_{2N-2})] \end{pmatrix},$$

$$\mathbf{M}_{2N} = \begin{pmatrix} 1 & -m_{2N}^*(x_{2N} - x_{2N-1}) \\ 0 & 1 \end{pmatrix},$$

$$k_1 = k_3 = \cdots = k_{2N-1} = k_{2N+1} = \sqrt{\frac{2m_j^* E}{\hbar^2}}, j = 1, 3, \cdots, 2N-1, 2N+1,$$

$$m_1^* = m_3^* = \cdots = m_{2N-1}^* = m_{2N+1}^*,$$

$$k_2 = k_4 = \cdots = k_{2N-2} = k_{2N} = 0, j = 2, 4, \cdots, 2N-2, 2N,$$

$$m_2^* = m_4^* = \cdots = m_{2N-2}^* = m_{2N}^*,$$

$$\text{令 } \mathbf{M} = \mathbf{M}_2 \times \mathbf{M}_3 \times \cdots \times \mathbf{M}_{2N-1} \times \mathbf{M}_{2N} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}.$$

综上可得 $E = v_0$ 时的透射系数:

$$T = \frac{4}{H_{11}^2 + \left(\frac{k_{2N+1}^*}{m_{2N+1}^*} H_{12}\right)^2 + \left(\frac{1}{\frac{k_1^*}{m_1^*}} H_{21}\right)^2 + H_{22}^2 + 2H_{11}H_{22} - 2H_{12}H_{21}}.$$

(3) $E < v_0$

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} e^{ik_1 x_1} & 0 \\ 0 & e^{-ik_1 x_1} \end{pmatrix}^{-1} \times \begin{pmatrix} 1 & 1 \\ i\frac{k_1^*}{m_1^*} & -i\frac{k_1^*}{m_1^*} \end{pmatrix}^{-1} \times \mathbf{M}_2 \times \mathbf{M}_3 \times \cdots \times \mathbf{M}_{2N-1} \times \mathbf{M}_{2N} \times$$

$$\begin{pmatrix} 1 & 1 \\ i\frac{k_{2N+1}^*}{m_{2N+1}^*} & -i\frac{k_{2N+1}^*}{m_{2N+1}^*} \end{pmatrix} \times \begin{pmatrix} e^{ik_{2N+1} x_{2N+1}} & 0 \\ 0 & e^{-ik_{2N+1} x_{2N+1}} \end{pmatrix} \times \begin{pmatrix} A_{2N+1} \\ B_{2N+1} \end{pmatrix},$$

其中:

$$\mathbf{M}_2 = \begin{pmatrix} \cosh[k_2(x_2 - x_1)] & -\frac{1}{\frac{k_2^*}{m_2^*}} \sinh[k_2(x_2 - x_1)] \\ -\frac{k_2^*}{m_2^*} \sinh[k_2(x_2 - x_1)] & \cosh[k_2(x_2 - x_1)] \end{pmatrix},$$

$$\mathbf{M}_3 = \begin{pmatrix} \cos[k_3(x_3 - x_2)] & -\frac{1}{\frac{k_3^*}{m_3^*}} \sin[k_3(x_3 - x_2)] \\ \frac{k_3^*}{m_3^*} \sin[k_3(x_3 - x_2)] & \cos[k_3(x_3 - x_2)] \end{pmatrix},$$

\vdots

$$\mathbf{M}_{2N-1} = \begin{pmatrix} \cos[k_{2N-1}(x_{2N-1} - x_{2N-2})] & -\frac{1}{\frac{k_{2N-1}^*}{m_{2N-1}^*}} \sin[k_{2N-1}(x_{2N-1} - x_{2N-2})] \\ \frac{k_{2N-1}^*}{m_{2N-1}^*} \sin[k_{2N-1}(x_{2N-1} - x_{2N-2})] & \cos[k_{2N-1}(x_{2N-1} - x_{2N-2})] \end{pmatrix},$$

$$M_{2N} = \begin{pmatrix} \cosh[k_{2N}(x_{2N} - x_{2N-1})] & -\frac{1}{\frac{k_{2N}^*}{m_{2N}^*}} \sinh[k_{2N}(x_{2N} - x_{2N-1})] \\ -\frac{k_{2N}^*}{m_{2N}^*} \sinh[k_{2N}(x_{2N} - x_{2N-1})] & \cosh[k_{2N}(x_{2N} - x_{2N-1})] \end{pmatrix}.$$

$$k_1 = k_3 = \cdots = k_{2N-1} = k_{2N+1} = \sqrt{\frac{2m_j^* E}{\hbar^2}}, j = 1, 3, \cdots, 2N-1, 2N+1,$$

$$m_1^* = m_3^* = \cdots = m_{2N-1}^* = m_{2N+1}^*,$$

$$k_2 = k_4 = \cdots = k_{2N-2} = k_{2N} = \sqrt{\frac{2m_j^* (v_0 - E)}{\hbar^2}}, j = 2, 4, \cdots, 2N-2, 2N,$$

$$m_2^* = m_4^* = \cdots = m_{2N-2}^* = m_{2N}^*.$$

$$\text{令 } M = M_2 \times M_3 \times \cdots \times M_{2N-1} \times M_{2N} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}.$$

综上可得 $E < v_0$ 时的透射系数:

$$T = \frac{4}{H_{11}^2 + \left(\frac{k_{2N+1}^*}{m_{2N+1}^*} H_{12}\right)^2 + \left(\frac{1}{\frac{k_1^*}{m_1^*}} H_{21}\right)^2 + H_{22}^2 + 2H_{11}H_{22} - 2H_{12}H_{21}}.$$

2 计算结果和分析

(1) 有效质量的影响

由图2知:随着有效质量的增大,产生共振透射的共振能量向低能量方向移动,各共振能量之间的间距随着有效质量的增大而减小,且势阱中的有效质量对共振能量的影响起主要作用.

(2) 势垒宽度的影响

由图3知:随着势垒宽度的增大,逐渐形成微带、微带的宽度衰减、微带之间的间距逐渐增大,微带逐渐转变为一个透射峰.同时当势垒宽度增大到某一个值后,低能量位置的透射系数随势垒宽度的增大逐渐减小、共振透射峰消失,在低能量位置不再发生共振透射,高能量位置的微带变化比低能量位置的微带变化慢.

(3) 势垒个数的影响

由图4知:随着势垒个数的增加,共振能量间距减小逐渐形成准连续微带,微带的宽度和微带之间的间距基本上不随势垒个数的变化而变化.

对于 $N = 5$ 势垒结构来说,含有4个势阱,在低能量的位置出现4个峰,表明由于4个势阱之间的相互作用使最低能量态分裂成量子化能级.

同理对于 $N = j$ 势垒结构来说,含有 $(j - 1)$ 个势阱,在低能量位置会出现 $(j - 1)$ 个峰.

3 结语

利用一维薛定谔方程和转移矩阵推导了多势垒结构的透射系数的一般表达式,采用

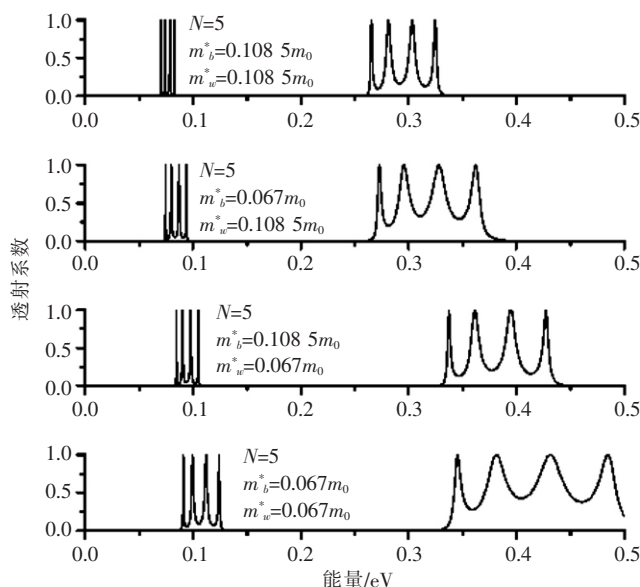


图2 五势垒结构的透射系数与能量的关系图.有效质量为参数,势垒宽度($a=2$ nm),势阱宽度($b=5$ nm),势垒高度($v_0=0.5$ eV)保持不变
Fig.2 Transmission coefficient as a function of incident electron energy for a five-barrier structure. The effective mass as a parameter. The barrier width ($a=2$ nm), the well width ($b=5$ nm), and the barrier height ($v_0=0.5$ eV) remain unchanged

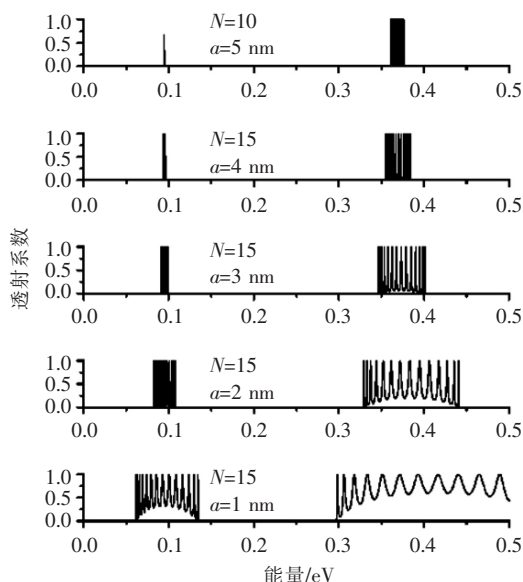


图3 十五势垒结构的透射系数与能量的关系图. 势垒宽度为参数, 有效质量($m_b^*=0.1085m_0$, $m_w^*=0.067m_0$), 势阱宽度($b=5\text{nm}$), 势垒高度($v_0=0.5\text{ eV}$)保持不变

Fig.3 Transmission coefficient as a function of incident electron energy for a fifteen-barrier structure. The barrier width as a parameter. The effective mass ($m_b^*=0.1085m_0$, $m_w^*=0.067m_0$), the well width ($b=5\text{nm}$), the barrier height ($v_0=0.5\text{ eV}$) remain unchanged

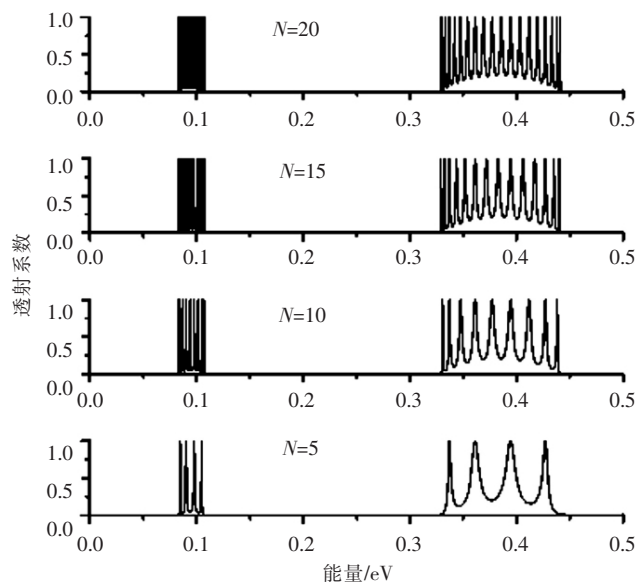


图4 多势垒结构透射系数与能量的关系图. 势垒个数为参数, 有效质量($m_b^*=0.1085m_0$, $m_w^*=0.067m_0$), 势垒宽度($a=2\text{ nm}$), 势阱宽度($b=5\text{nm}$), 势垒高度($v_0=0.5\text{ eV}$)保持不变

Fig.4 Transmission coefficient as a function of incident electron energy for a multi-barrier structure. The number of barriers as a parameter, the effective mass ($m_b^*=0.1085m_0$, $m_w^*=0.067m_0$), the barrier width ($a=2\text{ nm}$), the well width ($b=5\text{nm}$), the barrier height ($v_0=0.5\text{ eV}$) remain unchanged

GaAs/Ga_{1-x}Al_xAs 的参数, 计算了无偏压情况下 5 个、10 个、15 个、20 个势垒结构的透射系数, 并分析了势垒结构参数与共振能量之间的关系. 计算结果表明: (a) 发生共振透射的能量随有效质量 m_b^* 和 m_w^* 的增加逐渐向低能方向移动, 且 m_w^* 对共振能量的影响比 m_b^* 对其影响大. (b) 当势阱宽度一定时, 势垒宽度是影响准连续微带的宽度和微带之间间距的主要因素. 随着垒宽增大, 微带宽度衰减, 微带逐渐转变为一个透射峰, 微带之间的间距增大. (c) 势垒个数 (N) 与形成共振峰的个数 ($N-1$) 有直接关系. 随着势垒个数的增加, 共振能量间距减小, 逐渐形成准连续微带, 微带的宽度和微带之间的间距基本上不随势垒个数的变化而变化. 这些结果有利于我们对共振透射物理现象的理解及对实验和器件研究具有一定的参考和指导作用.

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