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Comment on "Effective-mass superlattice"

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In a paper by Sasaki [Phys. Rev. B **30**, 7016 (1984)], a new type of effective-mass superlattice (EMSL) was proposed and candidate materials for it were given. A band-structure determination for zero transverse wave vector k_t was presented as well. It was shown in our previously published papers that the flat potential (present in EMSL) is actually a special case that holds for singular k_t values (e.g., $k_t=0$), the potential varying periodically for all other k_t values. This fact influences the EMSL band structure and other parameters in a nontrivial way.

In a recent paper[1] Sasaki proposed and analyzed [within the effective-mass approximation (EMA)] the effective-mass superlattice (EMSL), having zero conduction-band-edge discontinuity and a periodic variation of the effective mass. Some material examples of EMSL's were presented in the paper as well.

However, in a previous paper[2] a general theory of superlattice (SL) band structure within the EMA was given. This theory included a zero conduction-band-edge discontinuity as a special case.

Starting from the effective-mass Schrödinger equation [Eq. (1) in (Ref. 2)]

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_{zz}}\frac{d\psi}{dz}\right]+U_{\rm eff}\psi=E\psi\ , \tag{1}$$

with the effective potential energy $U_{\rm eff}$ introduced in[2]

$$U_{\rm eff}(z)=U(z)+\frac{\hbar^2}{2}k_x^2\left[\frac{1}{m_{xx}}-\frac{m_{zz}}{m_{xz}^2}\right]+\hbar^2k_xk_y\left[\frac{1}{m_{xy}}-\frac{m_{zz}}{m_{xz}m_{yz}}\right]+\frac{\hbar^2}{2}k_y^2\left[\frac{1}{m_{yy}}-\frac{m_{zz}}{m_{yz}^2}\right]\ , \tag{2}$$

k_x and k_y being the transverse wave-vector components, m_{ij}^{-1} the components of the reciprocal effective-mass tensor and $U(z)$ the potential energy including band-edge discontinuities and the space-charge potential [both m_{ij}^{-1} and $U(z)$ vary periodically with the z coordinate], the E versus k_x,k_y,k_z relation can be derived for an arbitrary SL profile.

Analyzing Eq. (1) via the harmonic method, the conclusion that "the energy spectrum will have the band structure, if either the potential energy or the effective mass are space dependent, which means that even in the case of constant potential energy we have the allowed and the forbidden bands, since the effective potential energy is space dependent. Moreover, even when the effective potential energy $U_{\rm eff}$ is constant the spectrum again has the band structure due to the existence of extra space dependence of the effective mass," was deduced,[2] which actually predicts the existence of bandlike structure in the case of Sakaki's EMSL, although such a structure was not proposed as a possible real semiconductor structure.

Considering a special case of a rectangular SL with $U(z)=0$ and isotropic effective masses m_1 and m_2, the following expression for energy versus wave vector k_z can be derived as a special case of Eq. (6) in[3]

$$-\frac{r^2k_2^2+k_1^2}{2k_1k_2r}\sin(k_1d_1)\sin(k_2d_2)+\cos(k_1d_1)\cos(k_2d_2)=\cos(k_zd)\ , \tag{3}$$

r being the effective mass ratio m_1/m_2, d_1 and d_2 the layer thicknesses ($d=d_1+d_2$ is the SL period and k_1 and k_2 are given by $\hbar^2k_{1,2}^2=2Em_{1,2}-\hbar^2k_t^2$. Obviously, Eq. (4a) in (Ref. 1) is identical with (3) for $k_t=0$, but not for $k_t\neq0$. Therefore, the effective-mass difference implies that $U_{\rm eff}$ (being the cause of the existence of minizones has different z dependence for different k_t values, which should be taken into account when solving (3). In fact, the special case of $k_t=0$ was treated in Ref. 1.

The greater the effective mass ratio [being up to 5.7 (Ref. 1)] the more pronounced will be this effect and it may be of importance in the calculation EMSL parameters (carrier concentration, etc.).

[1]Akio Sasaki, Phys. Rev. B **30**, 7016 (1984).

[2]V. Milanović and D. Tjapkin, Physica **121B**, 187 (1983).

[3]V. Milanović and D. Tjapkin, Phys. Status Solidi B **110**, 687 (1982).