Detailed Derivation of Schottky Defect Equilibrium

Illustration

- Here is the detailed solution of the Poisson equation for Schottky defects:

Poisson equation of the problem

$$\boxed{\Delta V(\vec{r}) = -\frac{4\pi e N}{\epsilon\epsilon_0} \cdot \left\{ \exp\left[\frac{-(h^- + eV(\vec{r}))}{kT}\right] - \exp\left[\frac{-(h^+ - eV(\vec{r}))}{kT}\right]\right\}} \tag{1}$$

$$\Delta V(\vec{r}) = -\frac{4\pi e N}{\epsilon\epsilon_0} \cdot \left\{ \exp\left[\frac{-h^- - eV(\vec{r}) + \frac{h^+}{2} - \frac{h^+}{2}}{kT}\right] - \exp\left[\frac{-h^+ + eV(\vec{r}) + \frac{h^-}{2} - \frac{h^-}{2}}{kT}\right]\right\} \tag{2}$$

$$\begin{aligned} \Delta V(\vec{r}) \;=\; & -\frac{4\pi e N}{\epsilon\epsilon_0} \cdot \left\{ \exp\left[\frac{-eV(\vec{r}) + \frac{h^+}{2} - \frac{h^-}{2} - \frac{h^+}{2} - \frac{h^-}{2}}{kT}\right] \right. \\ & \left. - \exp\left[\frac{eV(\vec{r}) - \frac{h^+}{2} + \frac{h^-}{2} - \frac{h^+}{2} - \frac{h^-}{2}}{kT}\right]\right\} \end{aligned} \tag{3}$$

$$\begin{aligned} \Delta V(\vec{r}) \;=\; & -\frac{4\pi e N}{\epsilon\epsilon_0} \cdot \left\{ \exp\left[\frac{-eV(\vec{r}) + \frac{h^+}{2} - \frac{h^-}{2}}{kT}\right] \cdot \exp\left[-\frac{\frac{1}{2}(h^+ + h^-)}{kT}\right] \right. \\ & \left. - \exp\left[\frac{eV(\vec{r}) - \frac{h^+}{2} + \frac{h^-}{2}}{kT}\right] \cdot \exp\left[-\frac{\frac{1}{2}(h^+ + h^-)}{kT}\right]\right\} \end{aligned} \tag{4}$$

With $\boxed{v(\vec{r}) = \frac{eV(\vec{r}) - \frac{h^+}{2} + \frac{h^-}{2}}{kT}}$, (5)

follows

$$\Delta V(\vec{r}) = -\frac{4\pi e N}{\epsilon\epsilon_0} \cdot 2 \cdot \exp\left[-\frac{\frac{1}{2}(h^+ + h^-)}{kT}\right] \cdot \frac{1}{2}\left[\exp(-v(\vec{r})) - \exp(+v(\vec{r}))\right] \tag{6}$$

$$\boxed{\Delta V(\vec{r}) = +\frac{8\pi e N}{\epsilon\epsilon_0} \cdot \exp\left[-\frac{\frac{1}{2}(h^+ + h^-)}{kT}\right] \cdot \sinh(v(\vec{r}))} \tag{7}$$

Multiplication with e/kT and using eq. 5 gives

$$\frac{e}{kT} \cdot \Delta V(\vec{r}) = \Delta v(\vec{r}) = \frac{8\pi e^2 N}{\epsilon\epsilon_0 kT} \cdot \exp\left[-\frac{\frac{1}{2}(h^+ + h^-)}{kT}\right] \cdot \sinh(v(\vec{r})) \tag{8}$$

With $\boxed{\chi^2 = \frac{8\pi e^2 N}{\epsilon\epsilon_0 kT} \cdot \exp\left[-\frac{\frac{1}{2}(h^+ + h^-)}{kT}\right]}$ (9)

we obtain finally $\boxed{\Delta v(\vec{r}) = \chi^2 \sinh(v(\vec{r}))}$ (10)

1