

Detailed Derivation of Schottky Defect Equilibrium

Illustration

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

Poisson equation of the problem

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

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

$$\Delta V(\vec{r}) = -\frac{4\pi eN}{\epsilon\epsilon_0} \cdot \left\{ \exp\left[\frac{-eV(\vec{r}) + \frac{h^+}{2} - \frac{h^-}{2} - \frac{h^+}{2} - \frac{h^-}{2}}{kT}\right] - \exp\left[\frac{eV(\vec{r}) - \frac{h^+}{2} + \frac{h^-}{2} - \frac{h^+}{2} - \frac{h^-}{2}}{kT}\right] \right\} \quad (3)$$

$$\Delta V(\vec{r}) = -\frac{4\pi eN}{\epsilon\epsilon_0} \cdot \left\{ \exp\left[\frac{-eV(\vec{r}) + \frac{h^+}{2} - \frac{h^-}{2}}{kT}\right] \cdot \exp\left[-\frac{\frac{1}{2}(h^+ + h^-)}{kT}\right] - \exp\left[\frac{eV(\vec{r}) - \frac{h^+}{2} + \frac{h^-}{2}}{kT}\right] \cdot \exp\left[-\frac{\frac{1}{2}(h^+ + h^-)}{kT}\right] \right\} \quad (4)$$

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

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

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

Multiplication with e/kT and using eq. 5 gives

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

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

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