

BaTiO₃ has a primitive cubic lattice and a basis with atoms having fractional coordinates

$$\text{Ba } 000, \quad \text{Ti } \frac{1}{2}\frac{1}{2}\frac{1}{2}, \quad \text{O } \frac{1}{2}\frac{1}{2}0, \frac{1}{2}0\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}$$

Show that the X-ray structure factor for the (00*l*) Bragg reflections is given by

$$F_{hkl} = f_{\text{Ba}} + (-1)^l f_{\text{Ti}} + [1 + 2(-1)^l] f_{\text{O}},$$

where f_{Ba} is the atomic form (scattering) factor for Ba, etc.

Calculate the ratio I_{002}/I_{001} , where I_{hkl} is the intensity of the X-ray diffraction from the (*hkl*) planes. You may assume that the atomic form factor is proportional to atomic number (*Z*), and neglect its dependence on the scattering vector. [$Z_{\text{Ba}} = 56$, $Z_{\text{Ti}} = 22$, $Z_{\text{O}} = 8$]