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Mechanochemical synthesis of nanoparticles by a dilution method: derivation of kinetic equations

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Let us consider the case [18] of $z = z_1^* = 13.5$. Reactions of reagent 1 and 2 particles occur at contacts between reagent 1 particles with $R_1 = R_M = 0.828\times10^{-4}$ cm and $R_1 = R_S = 0.45\times10^{-4}$ cm and reagent 2 particles with $R_2 = R_B = 1.25\times10^{-4}$ cm (Figure 4). To simplify calculations, it makes sense to assume that the mean size of octahedral and tetrahedral voids is [18]: $\langle R_M, R_S\rangle = R_{MS} = (6R_M + 12R_S) / 18 = 0.573\times10^{-4}$ cm and $R_{12} = R_{12}(z_1^*) = R_{MS}R_B / (R_{MS} + R_B) = 0.393\times10^{-4}$ cm. At $z = z_2^* = 6.86$, we have (Figure 4): $R_1 = R_2 = R_B$ and $R_{12} = R_{12}(z_2^*) = R_B / 2 = 0.625\times10^{-4}$ cm. At $W_n = 900$ cm s^{-1}, $\theta + \underline{\theta} = 1.81\times10^{-11}$ and $\theta_1 + \theta_2 = 3.29\times10^{-11}$ cm^2 dyn^{-1}, see refs. 26, 27 and Table 1, calculations for $s_{12}(n = 1)$ in (10) give $s_{12}(n = 1, z_1^*) = 3.1\times10^{-10}$ cm^2 and $s_{12}(n = 1, z_2^*) = 11.7\times10^{-10}$ cm^2.

Here, relative shear velocity
$w_t(z) = 0.57\rho^{0.3}(\theta+\underline{\theta})^{-1.2}(\theta_1+\theta_2)W_n^{0.6}\,[(\rho_1 l_2^3+\rho_2 l_1^3)/\rho_1\rho_2(l_1+l_2)^3]^{0.5} =$
$0.57\rho^{0.3}(\theta+\underline{\theta})^{-1.2}(\theta_1+\theta_2)W_n^{0.6}\,[C_w(z)]^{0.5}$;
$C_w(z_1^*) = (\rho_1 R_B^{-3}+\rho_2 R_{MS}^{-3})/\rho_1\rho_2(R_B^{-1}+R_{MS}^{-1})^3 = 0.16$ cm^3 g^{-1},
$C_w(z_2^*) = (\rho_1 R_B^{-3}+\rho_2 R_B^{-3})/\rho_1\rho_2(R_B^{-1}+R_B^{-1})^3 = (\rho_1 + \rho_2) / 8\rho_1\rho_2 = 0.063$ cm^3 g^{-1}; and $w_t(z_1^*) \approx 6900$ cm s^{-1}, $w_t(z_2^*) \approx 4300$ cm s^{-1};
$t_{12}(z) = 3.5\rho^{-0.1}(\theta+\underline{\theta})^{0.4}W_n^{-0.2}\,[\rho_1\rho_2(l_1+l_2) / (\rho_1 l_2^3 +\rho_2 l_1^3)]^{0.5} = 3.5\rho^{-0.1}(\theta+\underline{\theta})^{0.4}W_n^{-0.2}\,[C_t(z)]^{0.5} \sim t'_m(z) \sim t_m(z)$; and $C_t(z_1^*) = \rho_1\rho_2\,(R_B^{-1}+R_{MS}^{-1}) / (\rho_1 R_B^{-3}+\rho_2 R_{MS}^{-3}) = 0.55\times10^{-8}$ g cm^{-1}, $C_t(z_2^*)] = 2\,R_B^2\,\rho_1\rho_2 / (\rho_1 + \rho_2) = 4.93\times10^{-8}$ g cm^{-1}.
From equation (2) at $\xi_{12} = 0.8$, see refs. 8−10 and Figure 2: $B(z_1^*) = 540\times10^5$, $B(z_2^*) = 320\times10^5$ K s$^{-0.5}$; $\tau_m = (\Delta T_m / B\,\mathrm{iErfc}\,[0])^2$, where iErfc [*] is the tabulated function of the error integral (iErfc [0] = 0.5642) and $T_0 \approx 350$ K, $T_{cm} \approx T_{m2}$, and $T_{m2} - T_0 \approx \Delta T_{m2} = 350$ K, $\tau'_m = (\tau_{12} + \tau_m)^2 / 4\tau_m$, $\tau_{12}(z_1^*) = 2.7\times10^{-9}$ s and $\tau_{12}(z_2^*) \approx 8.0\times10^{-9}$ s; and $t'_m(z_1) - t_m(z_1) \approx 1.2\times10^{-8}$ s, $t'_m(z_2) - t_m(z_2) \approx 5.3\times10^{-8}$ s;
$c_{12} = (c_1 + c_2) / 2 = 3.4\times10^6$ erg g^{-1} K^{-1}, $H_{m12} =(H_{m1} + H_{m2}) / 2 = 14.2\times10^8$ erg g^{-1}; $\mu_{12} = (\mu_1\mu_2)^{0.5} = 0.016$ dyn s cm^{-2}; $y = (\tau'_m / \tau_m) - 1$, and $(z_1^*) \approx 80$, $y(z_2^*) \approx 140$; $h = \pi^{0.5}\,c_{12}\,\Delta T_{m2} / H_{m12} \approx 1.5$; $\iota(y, h)$ is the tabulated function in the theory of melting [28], and $\iota[y(z_1^*)=80, h=1.5] \approx \iota[y(z_2^*)=140, h=1.5] \approx 0.9$.