

the number of these crystals within the CSD $n((L^3 - \lambda^3)^{1/3}, t)$ and $n(\lambda, t)$. $D_{\text{agg}}(L)$ states that if an L size crystal agglomerates with any crystal (λ), an L size crystal disappears from the system.

2.2.5 Modeling Crystal Breakage

Fragmentation of crystals might occur in certain crystallization systems, and is a collective name for all particle disintegration mechanisms, including the breakage, attrition, de-agglomeration *etc.* While the breakage can be neglected in some systems, it might play key role in the formation of CSD in others, like the binary breakage of rod-like crystals, the attrition (collision induced secondary nucleation), de-agglomeration during dissolution *etc.* The proper modeling of these fragmentation mechanisms requires mechanistic models that involve crystalline properties (shape, density, Young modulus) and solvent properties (density, viscosity) as well as stirring properties (stirring energy, circulation time). Generally speaking, the smaller the specific power input, the smaller the fragmentation rates are, but the presentation of such a complex model is beyond the scope of this subsection and it can be found in the literature.^{13,16} Instead, the generally used empirical and semi-empirical breakage functions will be presented here.

The overall rate of breakage of a λ size crystal is described by the so-called selection function:

$$S(\lambda) = b_0 S_0(\lambda) \quad (2.17)$$

Where b_0 is the breakage rate constant, dependent of crystal size, shape and hydrodynamic conditions, but in practice it is often used as a fitting parameter. $S_0(\lambda)$ describes the size dependency of the selection function. Various empirical selection functions were successfully applied, which are summarized in the Table 2.5.^{15,17} These functions aim to capture the experimental observation that the larger crystals break up with higher probability. The tangent hyperbolic selection function explicitly involves a critical crystal size (L_{crit}), under which the crystals don't tend to break.

The daughter crystals, formed by the breakage, can have any size between zero and the parent size with the restriction that the volume must be

Table 2.5 Commonly used breakage selection functions.

Name	$S_0(\lambda)$
Constant	1
Power law	λ^k
Exponential	$\exp(k\lambda)$
Tangent hyperbolic	$\frac{1}{2} \left[\tanh \left[k(\lambda - L_{\text{crit}}) \right] + 1 \right]$