

Supplementary Materials

Article

Using the BWA (Bertaut-Warren-Averbach) method to optimize the technology of crystalline powders such as LiFePO₄

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1. Various types of particle size distributions

For spherical particles of diameter L, we use the following one-dimensional expressions for the Lognormal, Normal, Gamma, and Weibull distributions, respectively:

1. Lognormal

$$f_{LN}(L|\bar{L}, W) = \frac{1}{\sqrt{2\pi} W L} \exp\left(-\frac{(\ln L - \ln \bar{L})^2}{2 W^2}\right), \quad (1)$$

where \bar{L} is the mean of the lognormal distribution and W is its dispersion.

2. Normal

$$f_N(L|\bar{L}, W) = \frac{1}{\sqrt{2\pi} w} e^{-\frac{(L - \bar{L})^2}{w^2}}, \quad (2)$$

where \bar{L} is the mean of the normal distribution, w is its dispersion, and $W = \frac{w}{\bar{L}}$ is its normalization.

3. Gamma

$$f_G(L|a, b) = \frac{1}{b^a \Gamma(a)} L^{a-1} e^{-\frac{L}{b}} \quad , \quad (3)$$

where a – shape parameter, b – scale parameter.

4. Weibull

$$f_W(L|\lambda, k) = k \lambda^{-k} L^{k-1} e^{-\left(\frac{L}{\lambda}\right)^k} \quad (4)$$

where a – scale parameter, b – shape parameter.

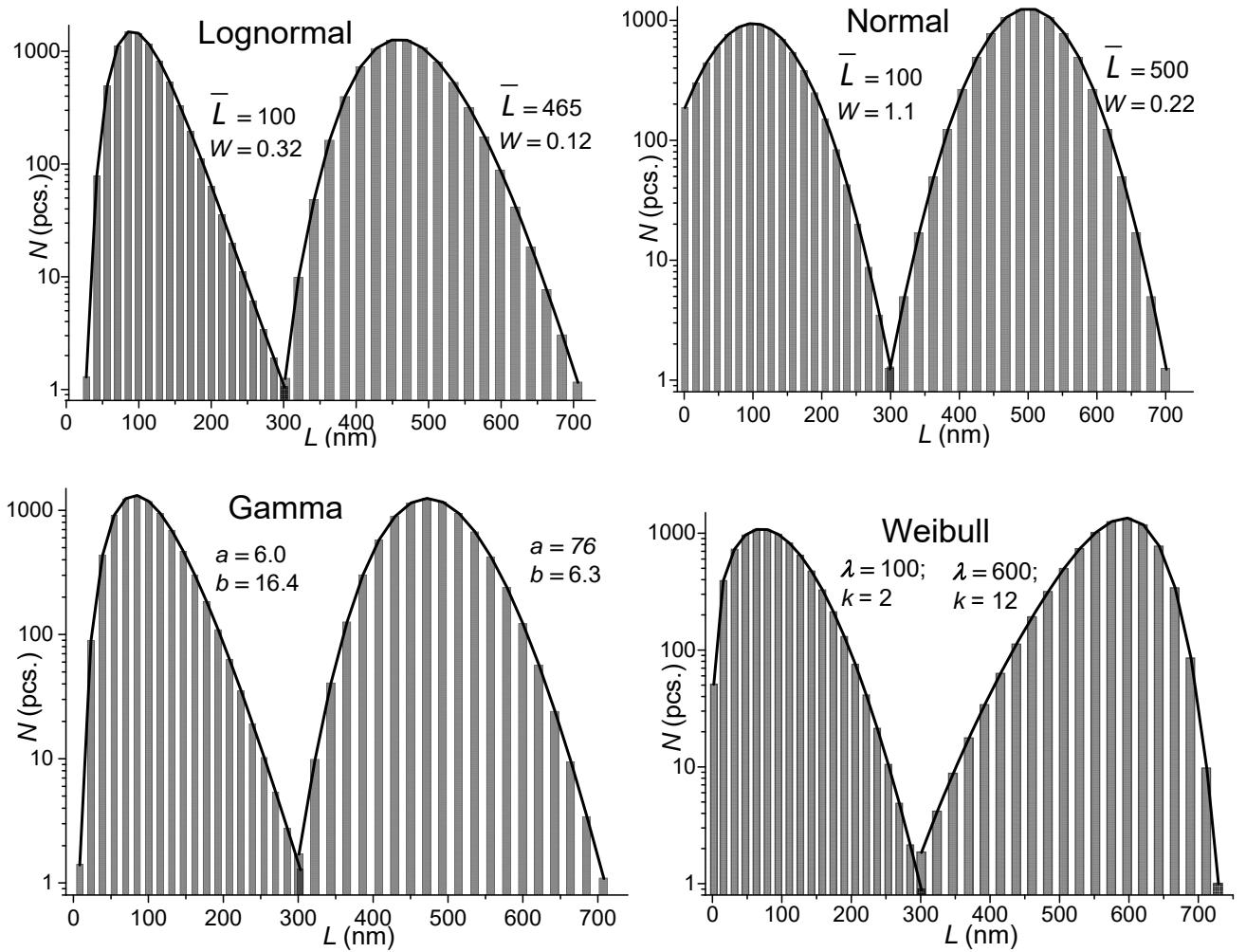


Figure S1. Digitization of 8000 particles and approximation by 20 bit histograms of distributions , their parameters are shown in the figures.

2. Checks and control of the stages of numerical calculations

Checks and control of the stages of numerical calculations on the example of a 3-dimensional 7-bit matrix of sizes lognormally distributed to ellipsoids, determination of sampling errors.

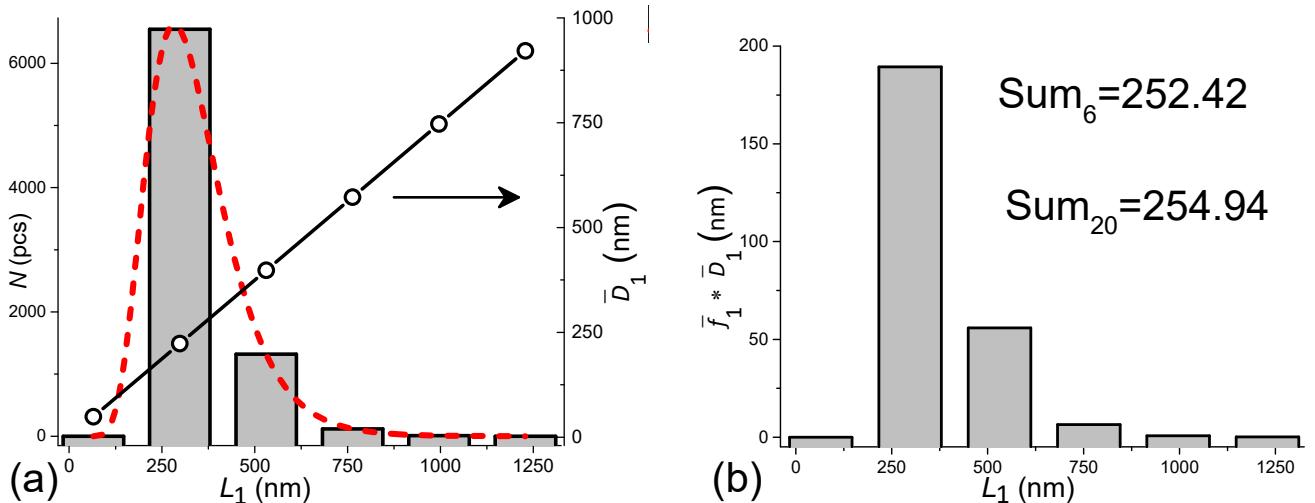


Figure S2. Ellipsoid calculation matrices with $\bar{L}_1 = \bar{L}_2 = \bar{L}_3 = 160$ nm , **(a)** 7-digit resolution of the sizes of ellipsoids; **(b)** correlation matrix, $W_1=0.5$, $r_{12} = r_{13} = r_{23} = r = 0.5$.

3. Examples of rows of 6-bit matrices for calculating the Lognormal distribution

Verification of the results of numerical calculations for the digitization of 8000 particles consists of the analysis of numerical values placed in rows, columns and position in the column of the corresponding size matrix.

922.	922.	922.	922.	922.	922.	922.	922.	922.	922.	922.	922.
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0.000629	1.92×10^{-6}	1.29×10^{-10}	3.73×10^{-14}	3.44×10^{-17}	7.52×10^{-20}
1.92×10^{-6}	0.000073	1.76×10^{-7}	4.84×10^{-10}	2.33×10^{-12}	1.87×10^{-14}
1.29×10^{-10}	1.76×10^{-7}	1.65×10^{-9}	1.07×10^{-11}	9.62×10^{-14}	1.27×10^{-15}
3.73×10^{-14}	4.84×10^{-10}	1.07×10^{-11}	1.19×10^{-13}	1.59×10^{-15}	2.86×10^{-17}
3.44×10^{-17}	2.33×10^{-12}	9.62×10^{-14}	1.59×10^{-15}	2.83×10^{-17}	6.41×10^{-19}
7.52×10^{-20}	1.87×10^{-14}	1.27×10^{-15}	2.86×10^{-17}	6.41×10^{-19}	1.73×10^{-20}
8.8×10^{-6}					
0.000333	0.0000333	8.02×10^{-7}	2.21×10^{-9}	1.06×10^{-11}	8.54×10^{-14}
$156.$	13.5	0.355	0.355	0.00889	0.000263
8.02×10^{-7}	13.5	4.55	0.282	0.0132	0.000639
2.21×10^{-9}	0.355	0.282	0.03	0.00208	0.000138
1.06×10^{-11}	0.00889	0.0132	0.00208	0.000193	0.0000161
8.54×10^{-14}	0.000263	0.000339	0.000138	0.0000161	1.6×10^{-6}
1.05×10^{-9}					
1.43×10^{-6}	1.43×10^{-6}	1.34×10^{-8}	8.7×10^{-11}	7.83×10^{-13}	1.03×10^{-14}
24.1	8.1	0.502	0.0235		0.00114
1.34×10^{-8}	8.1	10.6	0.136		0.0108
8.7×10^{-11}	0.502	1.55	0.0505		0.00548
7.83×10^{-13}	0.0235	0.136	0.00878		0.0012
1.03×10^{-14}	0.00114	0.0108	0.00548		0.000195
4.37×10^{-13}					
5.67×10^{-9}	5.67×10^{-9}	1.25×10^{-10}	1.4×10^{-12}	1.86×10^{-14}	3.35×10^{-16}
0.911	0.722	0.722	0.0767	0.00534	0.000353
1.25×10^{-10}	0.722	2.23	0.558	0.0727	0.00789
1.4×10^{-12}	0.0767	0.558	0.24	0.0464	0.00687
1.86×10^{-14}	0.00534	0.0727	0.0464	0.012	0.00223
3.35×10^{-16}	0.000353	0.00789	0.00687	0.00223	0.000496
5.26×10^{-16}					
3.55×10^{-11}	3.55×10^{-11}	1.47×10^{-12}	2.43×10^{-14}	4.33×10^{-16}	9.79×10^{-18}
0.0297	0.0441	0.00696	0.000646		0.0000537
1.47×10^{-12}	0.0441	0.255	0.0948	0.0165	0.00225
2.43×10^{-14}	0.00696	0.0948	0.0605	0.0156	0.0029
4.33×10^{-16}	0.000646	0.0165	0.0156	0.00537	0.00126
9.79×10^{-18}	0.0000537	0.00225	0.0029	0.00126	0.000352
1.42×10^{-18}					
3.52×10^{-13}	3.52×10^{-13}	2.39×10^{-14}	5.39×10^{-16}	1.21×10^{-17}	3.27×10^{-19}
0.00108	0.00264	0.000568	0.0000663		6.59×10^{-6}
2.39×10^{-14}	0.00264	0.025	0.0127	0.00277	0.000452
5.39×10^{-16}	0.000568	0.0127	0.0111	0.00358	0.000798
1.21×10^{-17}	0.0000663	0.00277	0.00358	0.00155	0.000434
3.27×10^{-19}	6.59×10^{-6}	0.000452	0.000798	0.000434	0.000145

(e)

Figure S3. Verification of the results of numerical calculations for the digitization of 8000 particles. **(a)** 3-dimensional 6-bit size matrix with 1 each for the minimum and maximum sizes of 65.2 and 1229 nm, respectively. **(b)** correlation matrix with $W_1=W_2=W_3=0.35$, $r_{12}=r_{13}=r_{23}=r=0.5$. **(c)** the matrix of the number of particles with given sizes, for example, with sizes $297.96 * 530.72 * 297.96$ we have with the number 484 placed in the 2nd row, 3rd column, 2nd number. **(d)** averaging the length of the ellipsoid columns along L_1 65.2 nm (upper left corner of the matrix (d)), check that it is indeed $65.2*3/4=48.9$ nm, and along L_1 1229 nm (lower right corner of the matrix (d)) , it is equal to $1229*3/4=922$ nm. **(e)** matrices of contributions to the average total column length.

4. Dependence of column length on digit number N

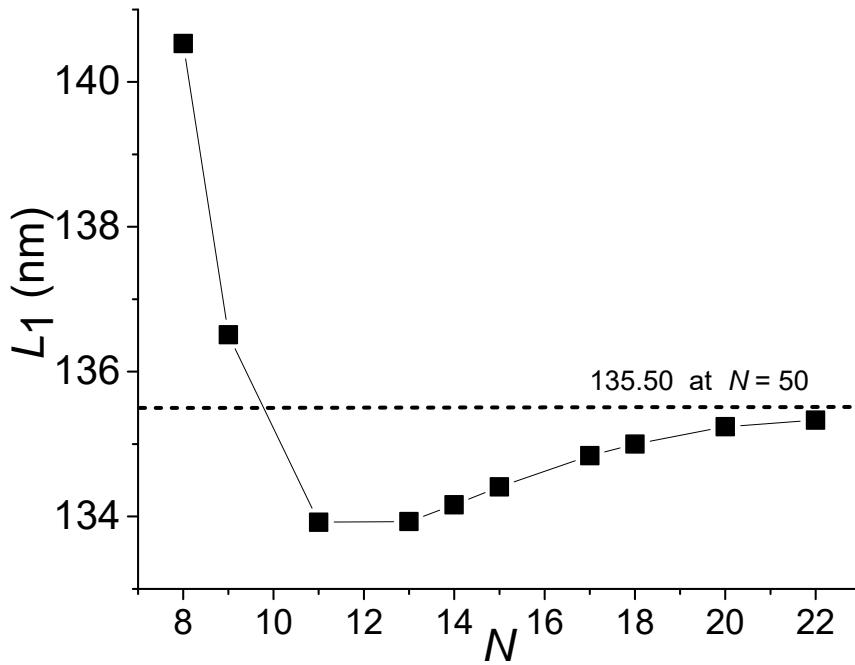


Figure S4. Dependence of column length on digit number N , averaged over 8000 ellipsoids, lognormally distributed with the parameters Figure S1. It can be seen from the figure that, relative to the asymptotic value, for the number of digits used in the work $N = 20$, the error in determining L_1 is 0.2%, and for the number of digits > 12 , the error in determining is less than 1%. The dotted line shows the value for a 50-bit matrix.

5. Comparison of curves with 20 and 30 histogram sizes

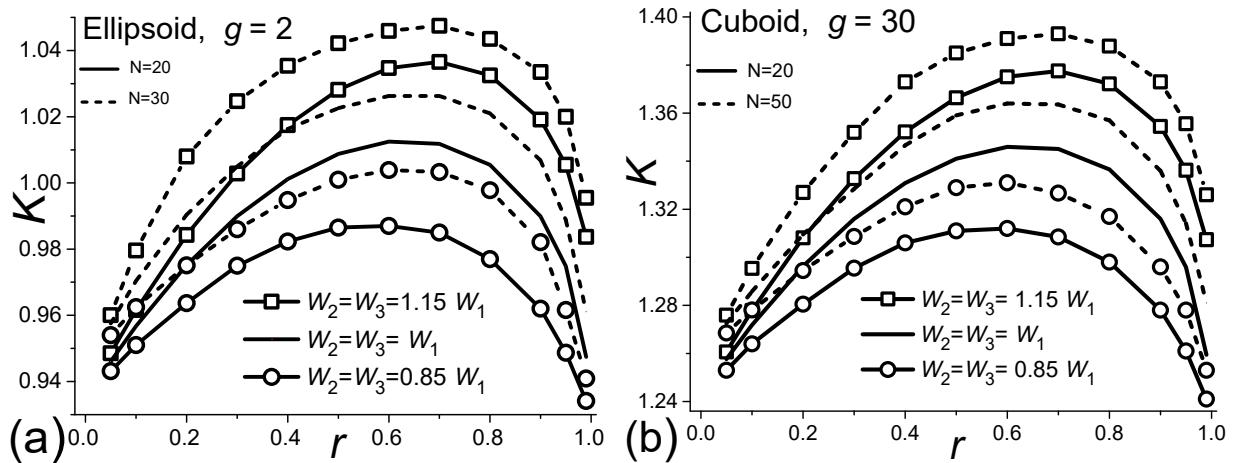


Figure S5. Comparison of curves with 20 and 30 histogram sizes. The calculation parameters are indicated in the caption to Figure 5 of article text.