Supplementary Information (SI) for Nanoscale.

Electronic Supporting Information Structural Classification of Ag and Cu Nanocrystals with Machine Learning

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CNA Signature List

In Table S1, we present the list of 32 combinations of CNA signatures used to build our feature set.

Table S1: Atomic CNA signatures for the most common environments observed in this study. C_N is the coordination number and in $\{i,j,k\}(\#)$, # is the number of bonds with $\{i,j,k\}$ indices.

Atom Type	C_N	$\{i,j,k\}(\#)$	$\{i,j,k\}(\#)$	$\{i,j,k\}(\#)$	$\{i,j,k\}(\#)$	$\{i,j,k\}(\#)$	$\{i,j,k\}(\#)$
FCC bulk	12	{4,2,1}(12)					
HCP bulk	12	{4,2,1}(6)	{4,2,2}(6)				
FCC{111} surface	9	{4,2,1} (3)	{3,1,1}(6)				
FCC vertex	6	{4,2,1}(1)	{3,1,1}(2)	{2,1,1}(2)	{2,0,0}(1)		
FCC {111}-{100} edge	7	{4,2,1}(2)	{3,1,1}(2)	{2,1,1}(3)			
FCC {111}-{111} edge	7	{4,2,1}(1)	{3,1,1}(4)	{2,0,0}(2)			
Ih spine	12	{4,2,2}(10)	{5,5,5}(2)				
Ih surface edge	8	{4,2,2}(2)	{3,2,2}(2)	{3,1,1}(4)			
Dh-Ih notch vertex	7	{4,2,2}(1)	{3,2,2}(1)	{3,1,1}(2)	{3,0,0}(1)	{2,0,0}(2)	
Dh notch edge	10	{4,2,2}(2)	{4,2,1}(2)	{3,1,1}(4)	{3,0,0}(2)		
twisted Ih surface edge	9	{4,2,2}(2)	{4,2,1}(2)	{3,2,2}(2)	{3,1,1}(2)	{2,1,1}(1)	
twisted Ih surface vertex	6	{4,2,2}(1)	{3,2,2}(1)	{3,1,1}(1)	{2,1,1}(1)	{2,0,0}(2)	
Ih center	12	{5,5,5}(12)					
FCC {100} surface	8	{4,2,1}(4)	{2,1,1}(4)				
Ih/Dh surface vertex	6	{5,5,5}(1)	{3,2,2}(5)				
Dh-Ih bulk 5-fold ring: 1	11	{4,2,2}(3)	{4,2,1}(2)	{4,3,3}(1)	{3,1,1}(3)	{3,2,2}(1)	{2,0,0}(1)
Dh-Ih bulk 5-fold ring: 2	11	{4,2,2}(4)	{4,2,1}(2)	{4,3,3}(1)	{3,1,1}(3)	{3,0,0}(1)	
Dh-Ih bulk 5-fold ring: 3	11	{4,2,2}(4)	{4,1,1}(1)	{3,1,1}(3)	{3,0,0}(1)	{2,0,0}(2)	
Dh-Ih bulk 5-fold ring: 4	11	{5,5,5}(1)	{4,2,2}(6)	{3,1,1}(2)	{3,2,2}(1)	{2,0,0}(1)	
Dh-Ih {111} surface	9	{4,1,1}(1)	{3,1,1}(8)				
Dh-Ih surface edge	8	{4,2,2}(1)	{3,2,2}(1)	{3,1,1}(5)	{2,0,0}(1)		
Dh-Ih {111}-{100} edge	7	{4,3,3}(1)	{3,2,2}(2)	{3,1,1}(2)	{2,0,0}(2)		
Dh-Ih surface vertex	6	{4,3,3}(1)	{3,2,2}(2)	{3,1,1}(2)	{2,0,0}(1)		
Twisted Ih surface edge vertex	8	{5,5,5}(1)	{4,2,2}(2)	{3,2,2}(3)	{2,0,0}(2)		
HCP $\{10\bar{1}1\}$ surface & edge anti-Mackay	8	{4,2,1}(1)	{3,1,1}(2)	{4,2,2}(2)	{2,0,0}(2)	{2,1,1}(1)	
HCP $\{10\bar{1}0\}$-$\{10\bar{1}1\}$ edge	7	{2,0,0}(1)	{2,1,1}(2)	{4,2,2}(1)	{4,2,1}(1)	{3,2,2}(1)	{3,1,1}(1)
sharp FCC edge between HCP islands	10	{3,1,1}(4)	{4,2,2}(4)	{4,3,3}(2)			
missing 5-fold vertex am surrounding atoms	7	{4,3,3}(1)	{2,1,1}(2)	{2,0,0}(2)	{4,2,2}(2)		
atoms around noncentral hole in Ih	11	{3,1,1}(4)	{4,2,1}(7)				
type 1	5	{2,0,0}(2)	{3,1,1}(2)	{2,1,1}(1)			
type 2	8	{3,1,1}(4)	{2,1,1}(1)	{4,2,1}(2)	{2,0,0}(1)		
type 3	12	{4,2,1}(5)	{4,2,2}(4)	{3,1,1}(2)	{4,1,1}(1)		

Ag Fraction of Atomic CNA Environments

In Figures S1 to S4, we present the fraction of atomic CNA environments for all 14 structural classes grouped by K-Means clustering, except for 3 classes relevant to FCC/SCSF, which were shown in the main text.

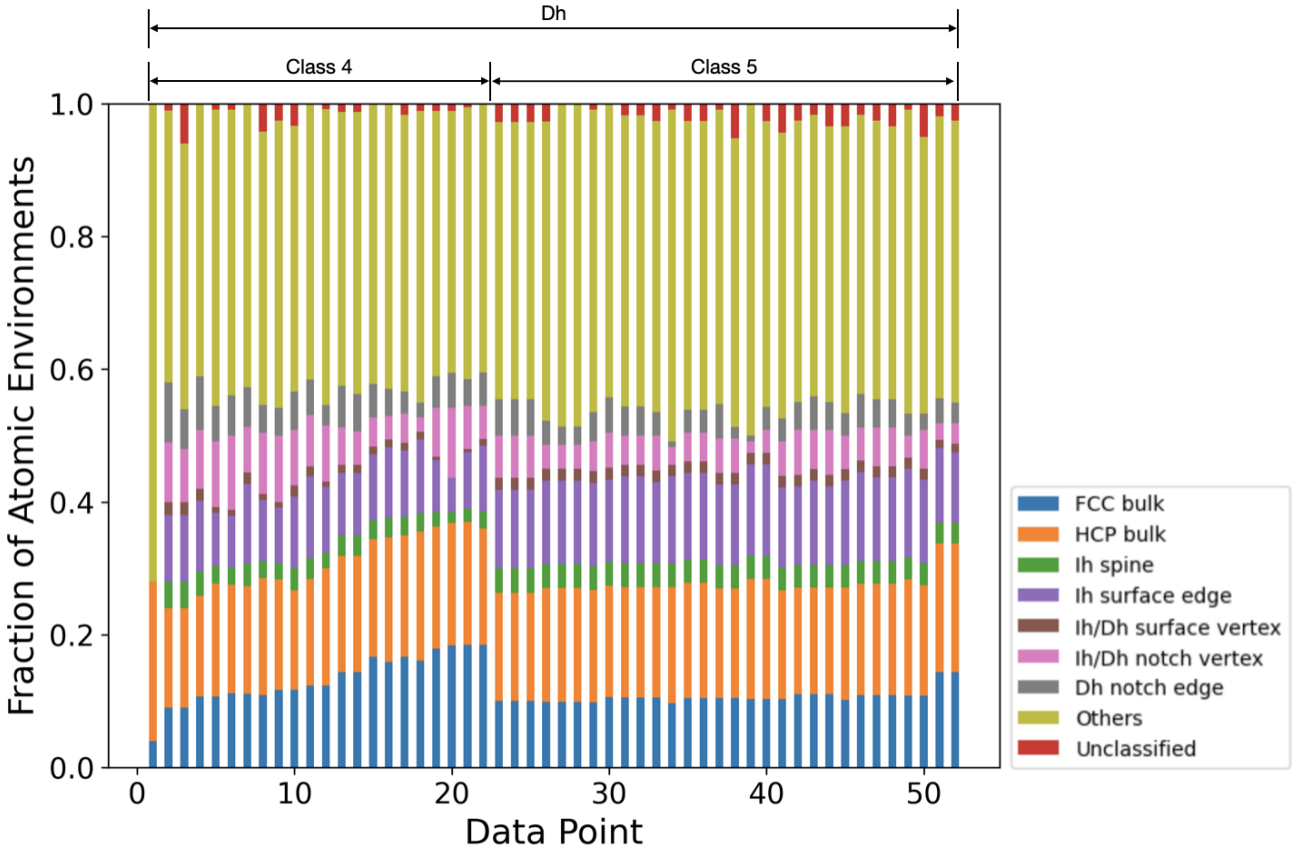

Figure S1: Fraction of atomic CNA environments (see Table S1) for the two Dh classes for Ag.

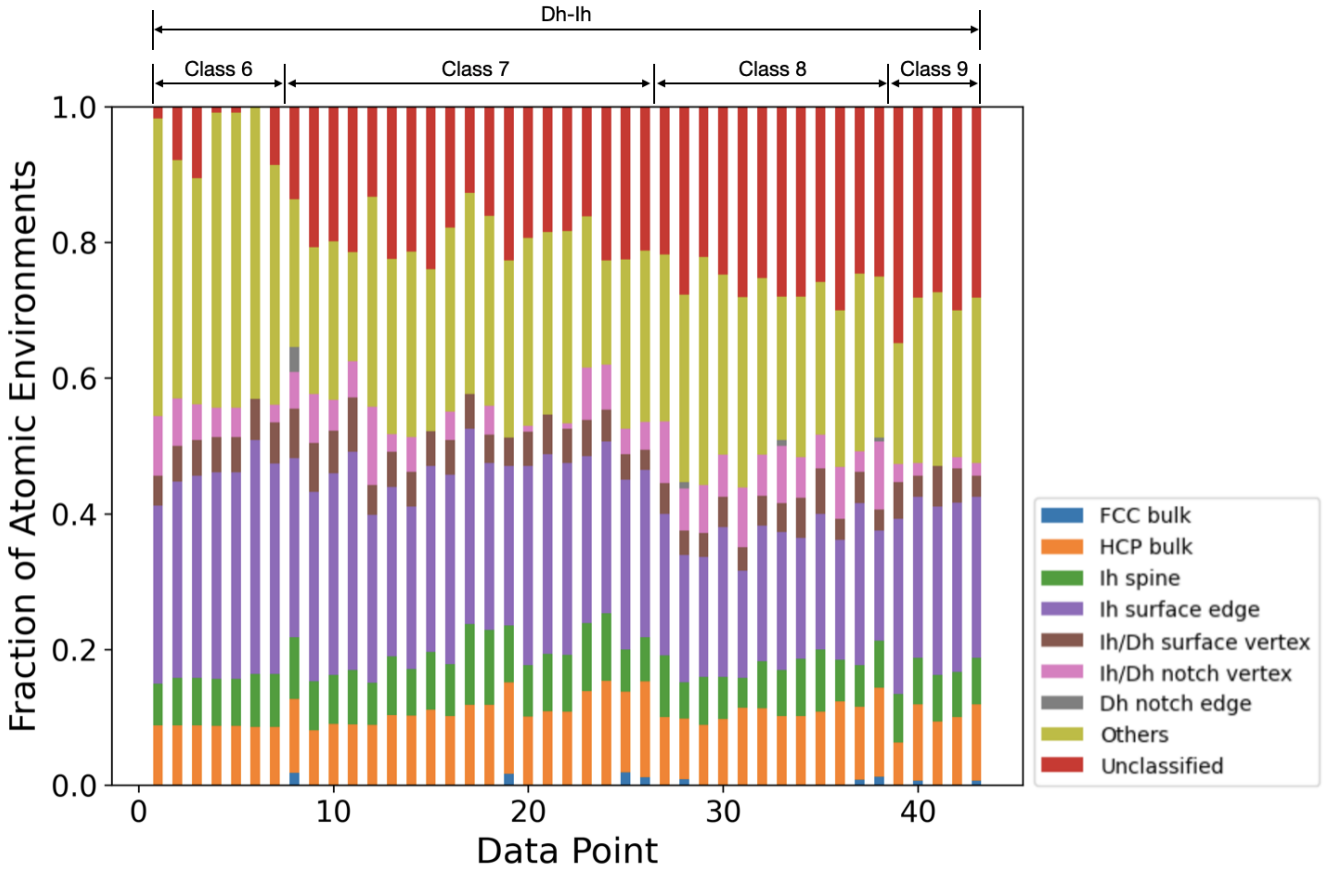

Figure S2: Fraction of atomic CNA environments (see Table S1) for the four Dh-Ih classes for Ag.

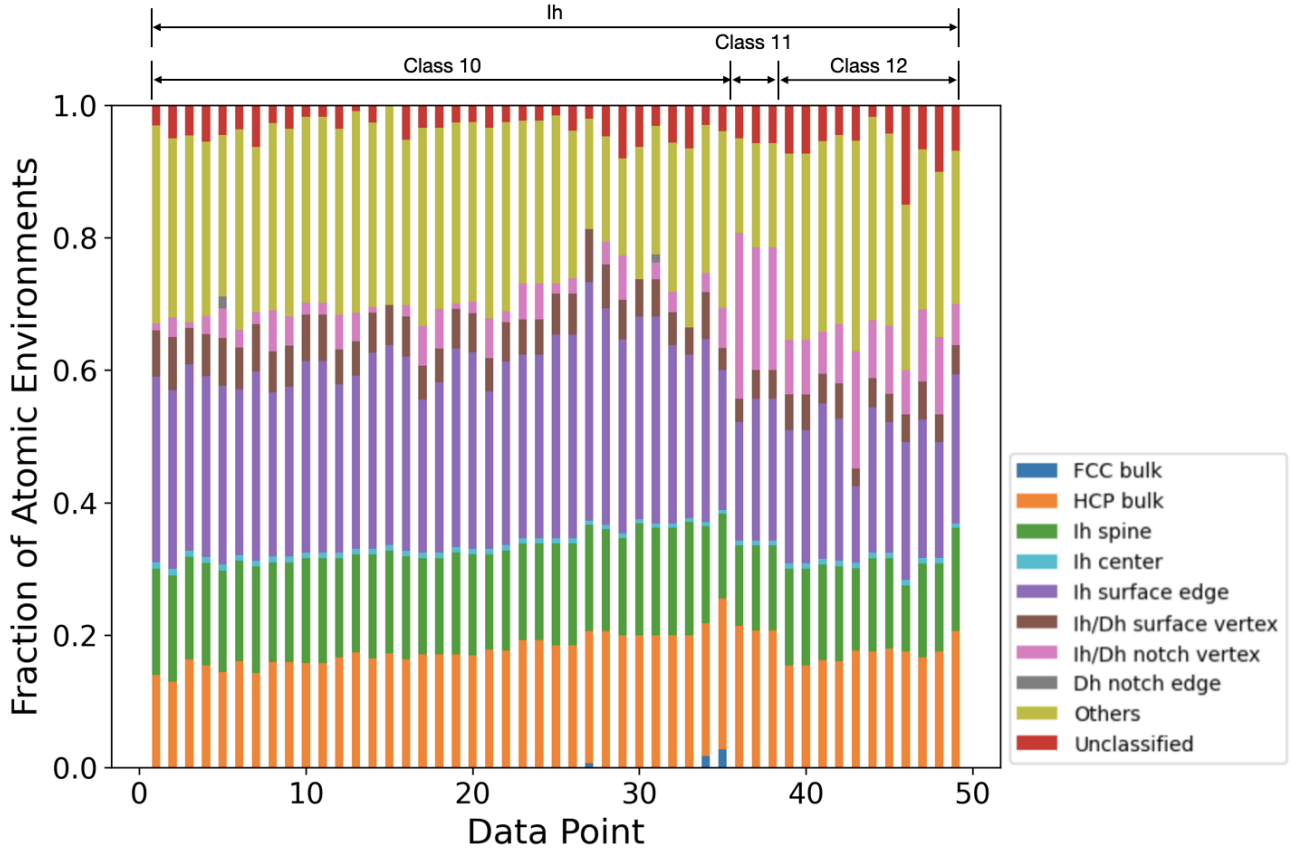

Figure S3: Fraction of atomic CNA environments (see Table S1) for the three Ih classes for Ag.

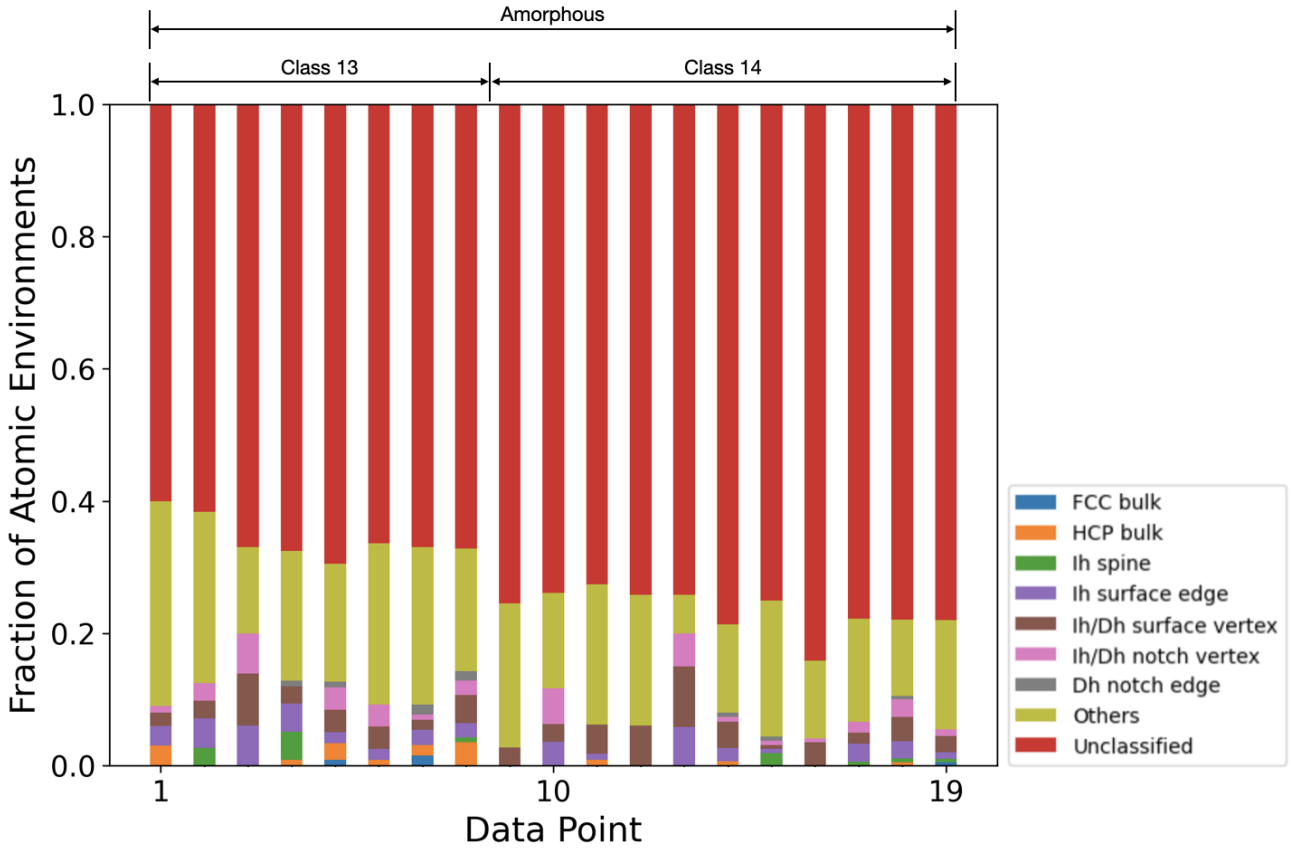

Figure S4: Fraction of atomic CNA environments (see Table S1) for the two Amorphous classes for Ag.

Cu Fraction of Atomic CNA Environments

In Figures S5 to S9, we present the fraction of atomic CNA environments for all 15 structural classes grouped by K-Means clustering.

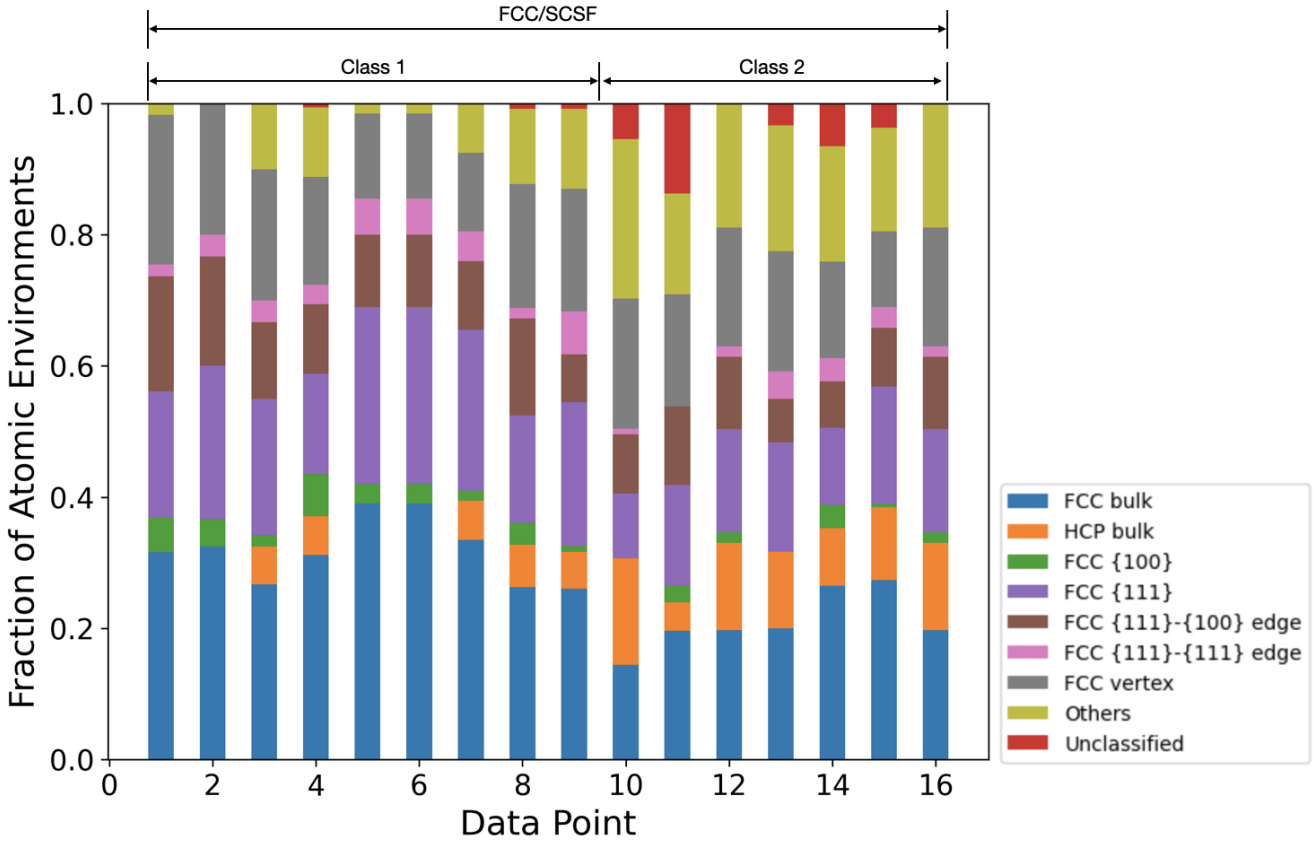

Figure S5: Fraction of atomic CNA environments (see Table S1) for the two FCC/SCSF classes for Cu.

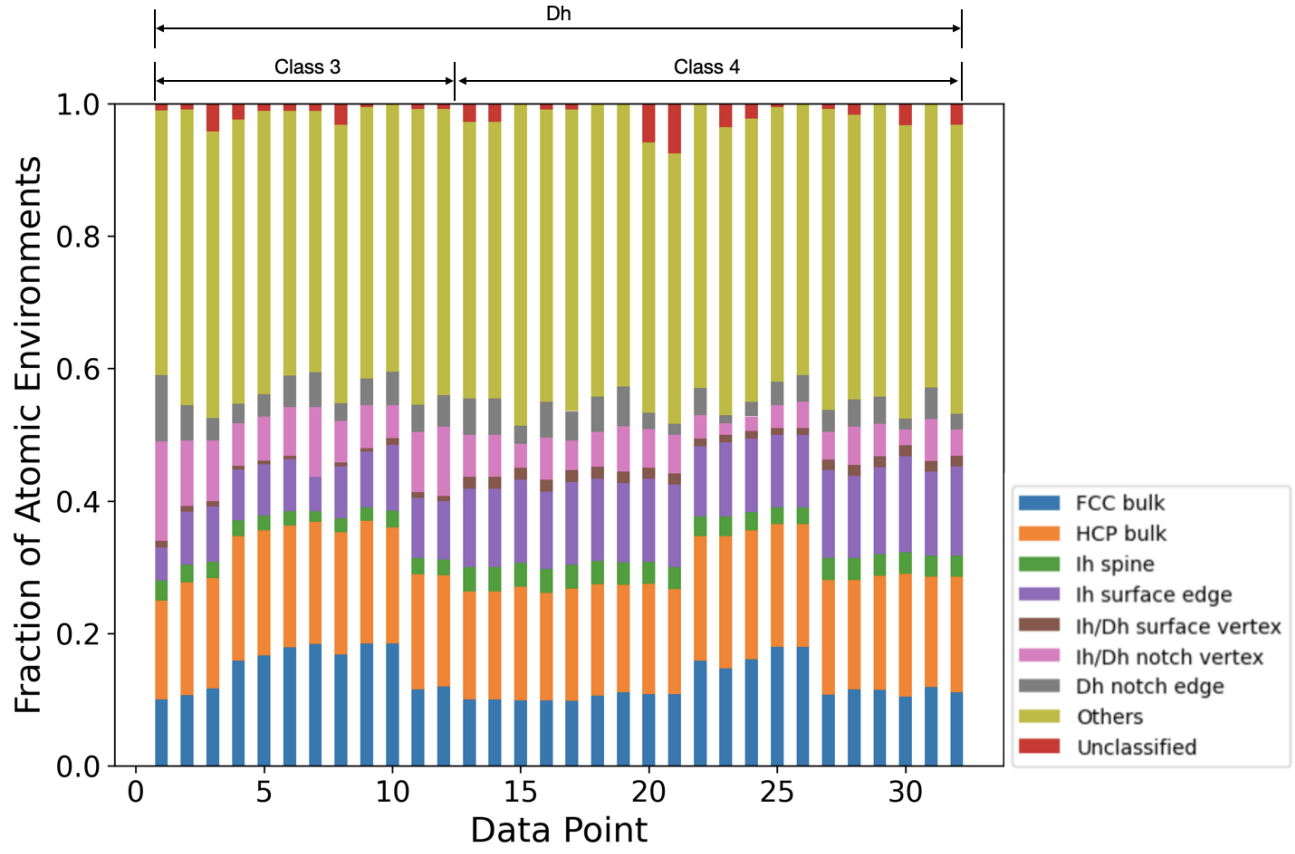

Figure S6: Fraction of atomic CNA environments (see Table S1) for the two Dh classes for Cu.

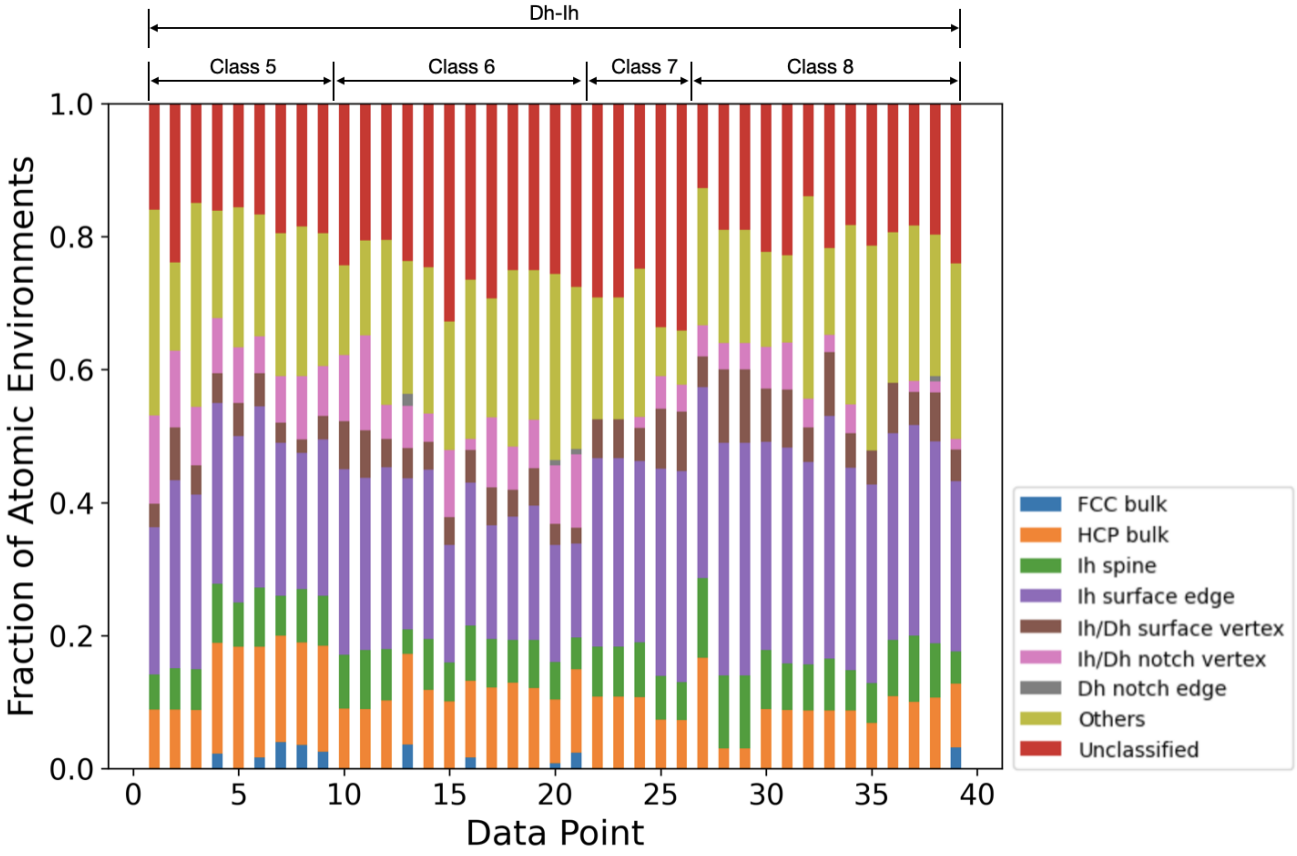

Figure S7: Fraction of atomic CNA environments (see Table S1) for the four Dh-Ih classes for Cu.

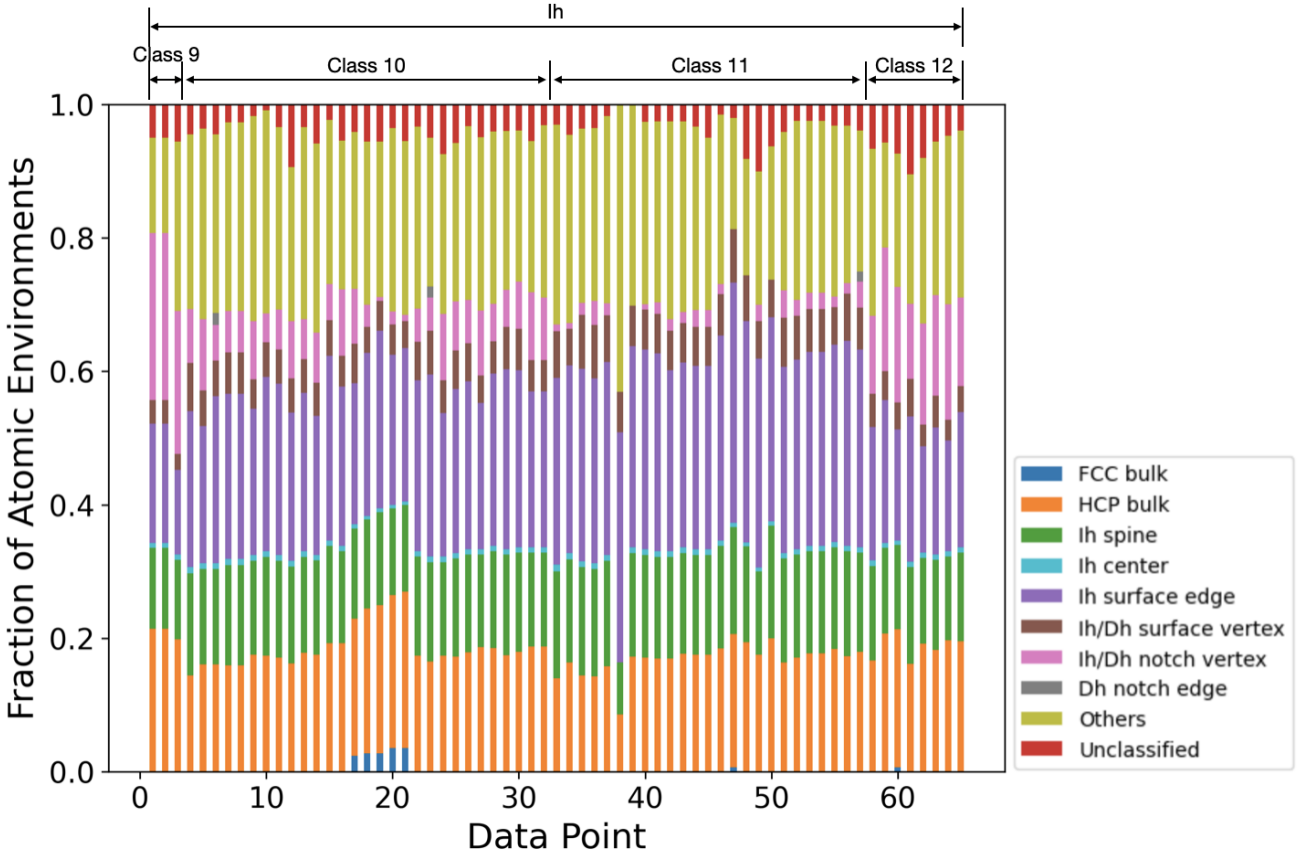

Figure S8: Fraction of atomic CNA environments (see Table S1) for the four Ih classes for Cu.

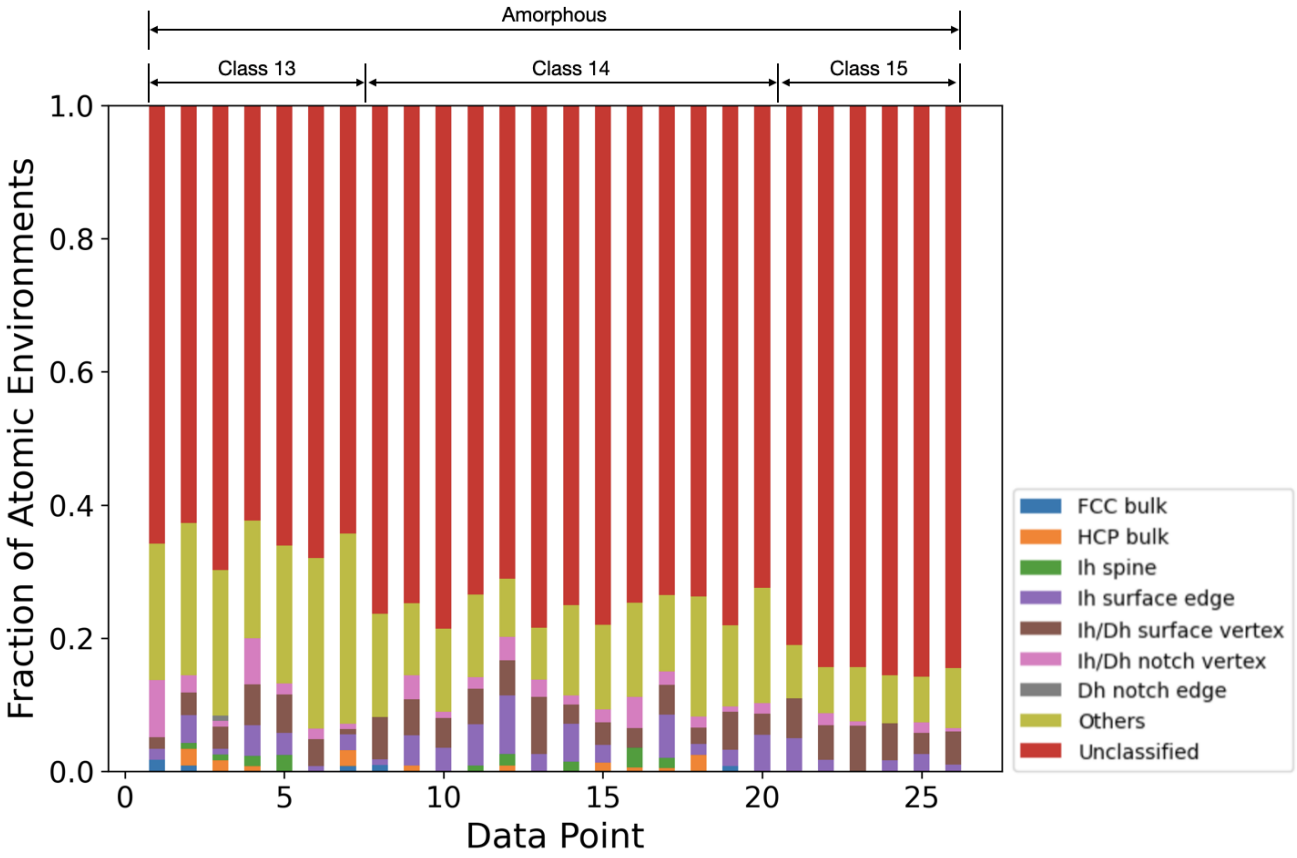

Figure S9: Fraction of atomic CNA environments (see Table S1) for the three Amorphous classes for Cu.