Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Proportional scaling molecular dynamics simulations of the wetting experiments of water droplets on ink-patterned printing paper

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Table S1. Square pattern structure and contact angle measurements. The width length *a* is the square side length of the ink pattern. The interval length *b* is the square interval length.

Sample code	Width length *a* (μm)	Interval length *b* (μm)	Contact angle (degree)
QW2I15	240	119	61.65
QW2I20	240	184	58.53
QW2I25	240	219	58.97
QW2I30	240	251	58.68
QW2I35	240	300	58.52
QW2I40	240	367	56.36
QW2I45	240	418	56.30
QW3I15	342	118	66.12
QW3I20	342	166	63.77
QW3I25	342	197	62.76
QW3I30	342	255	56.97
QW3I35	342	308	58.72
QW3I40	342	346	56.10
QW3I45	342	390	57.80
QW4I15	444	111	61.62
QW4I20	444	151	62.93
QW4I25	444	218	62.89
QW4I30	444	257	60.12
QW4I35	444	314	58.03
QW4I40	444	350	58.35
QW4I45	444	373	61.22
QW5I15	551	123	63.65
QW5I20	551	168	60.35
QW5I25	551	206	60.66
QW5I30	551	252	60.24
QW5I35	551	311	58.04
QW5I40	551	356	58.14
QW5I45	551	390	57.07

Table S2. Grid pattern structure and contact angle measurements. The width length *a* is the width of the grid ink pattern. The interval length *b* is the interval width of printing paper.

Sample code	Width length *a* (μm)	Interval length *b* (μm)	Contact angle (degree)
GH131V95	131	95	62.23
GH137V92	137	92	63.92
GH151V149	151	149	63.41
GH156V137	156	137	62.37
GH209V189	209	189	61.44
GH234V196	234	196	61.83
GH261V136	261	136	63.38
GH189V149	189	149	61.43
GH160V144	160	144	61.64
GH176V178	176	178	61.55
GH207V191	207	191	61.52
GH133V79	133	79	61.39
GH244V119	244	119	63.20
GH177V115	177	115	61.01
GH179V140	179	140	61.90
GH168V138	168	138	61.85
GH205V171	205	171	62.53
GH231V180	231	180	61.92
GH282V232	282	232	60.87
GH207V104	207	104	63.83
GH182V114	182	114	63.14
GH177V144	177	144	61.29
GH181V140	181	140	62.02
GH210V151	210	151	62.31
GH250V176	250	176	61.41
GH304V250	304	250	61.49
GH295V262	295	262	60.95

Table S3. Stripe pattern structure and contact angle measurements. The width length *a* is the width of the stripe ink pattern. The interval length *b* is the interval width of printing paper.

Sample code	Width length *a* (μm)	Interval length *b* (μm)	Contact angle (degree)
SW109I141	109	141	55.64
SW109I191	109	191	55.33
SW109I241	109	241	53.16
SW138I112	138	112	58.32
SW138I162	138	162	56.76
SW138I212	138	212	54.60
SW158I92	158	92	63.64
SW158I142	158	142	57.40
SW158I192	158	192	57.23
SW173I77	173	77	66.23
SW173I127	173	127	61.67
SW173I177	173	177	56.52
SW190I60	190	60	63.58
SW190I110	190	110	64.37
SW190I160	190	160	57.84
SW206I44	206	44	65.20
SW206I94	206	94	62.14
SW206I144	206	144	61.49
SW245I5	245	5	65.39
SW245I55	245	55	64.55
SW245I105	245	105	63.83

Grid and stripe pattern surface in MD simulation

For grid-pattern, the corresponding width of ink-patterned grid a is approximated in the range of 1.5 a_{Cu} to 4.0 a_{Cu}. The square interval length b is approximated in the range of 1.5 a_{Cu} to 3.5 a_{Cu}. Thus, there are 15 sets of grid patterns with different b/a combinations to be simulated (shown in Fig. S1).

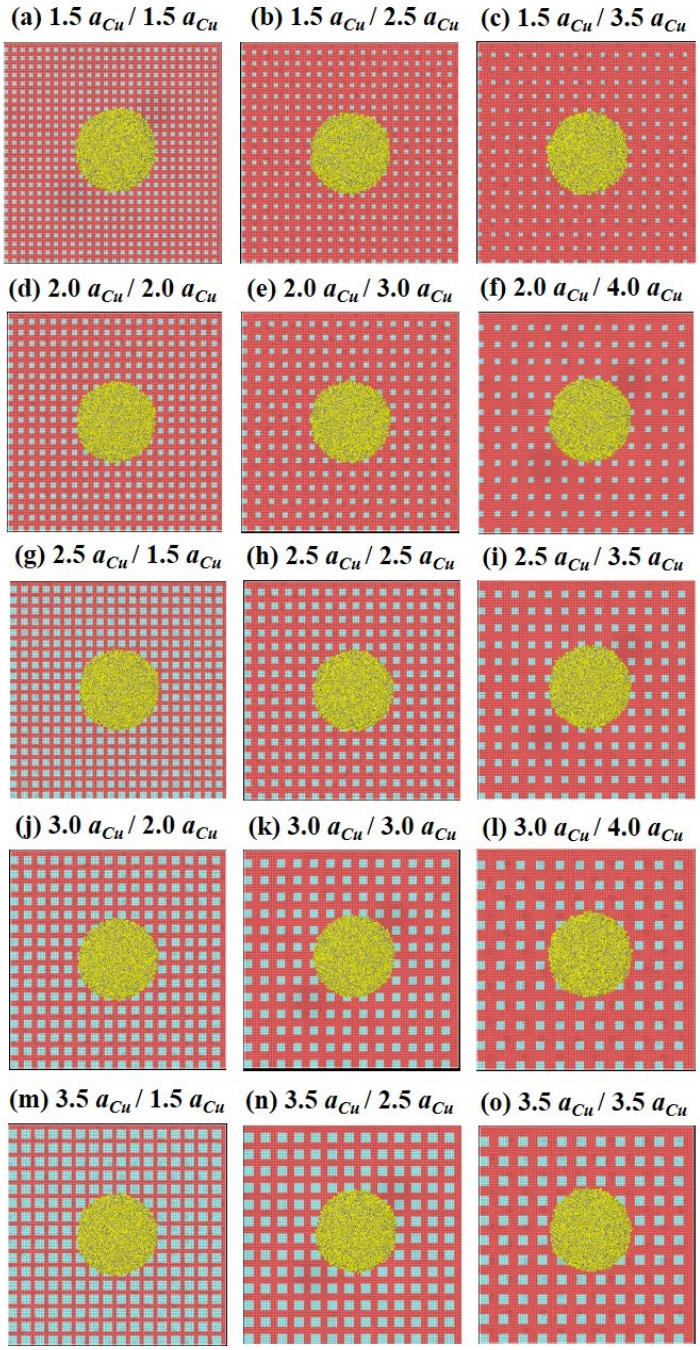

Fig. S1. Top view of ink grid-pattern surface and water droplet at the beginning of water droplet wetting MD simulation. The descriptions behind the (a-o) are b/a. The a is the width of the ink-patterned grid, and b is the square side length of the printing paper. The red atoms stand for the ink surface, and the azure atoms stand for the printing paper surface. The yellow and blue atoms stand for the oxygen and hydrogen atoms in water, respectively.

For stripe-pattern, the corresponding stripe width of ink-pattern a is approximately in the range of 1.5 a_{Cu} to 3.5 a_{Cu}. The stripe interval width of printing paper b is approximately in the range of 1.5 a_{Cu} to 4.0 a_{Cu}. Thus, there are 15 sets of grid patterns with different b/a combination to be simulated (shown in Fig. S2).

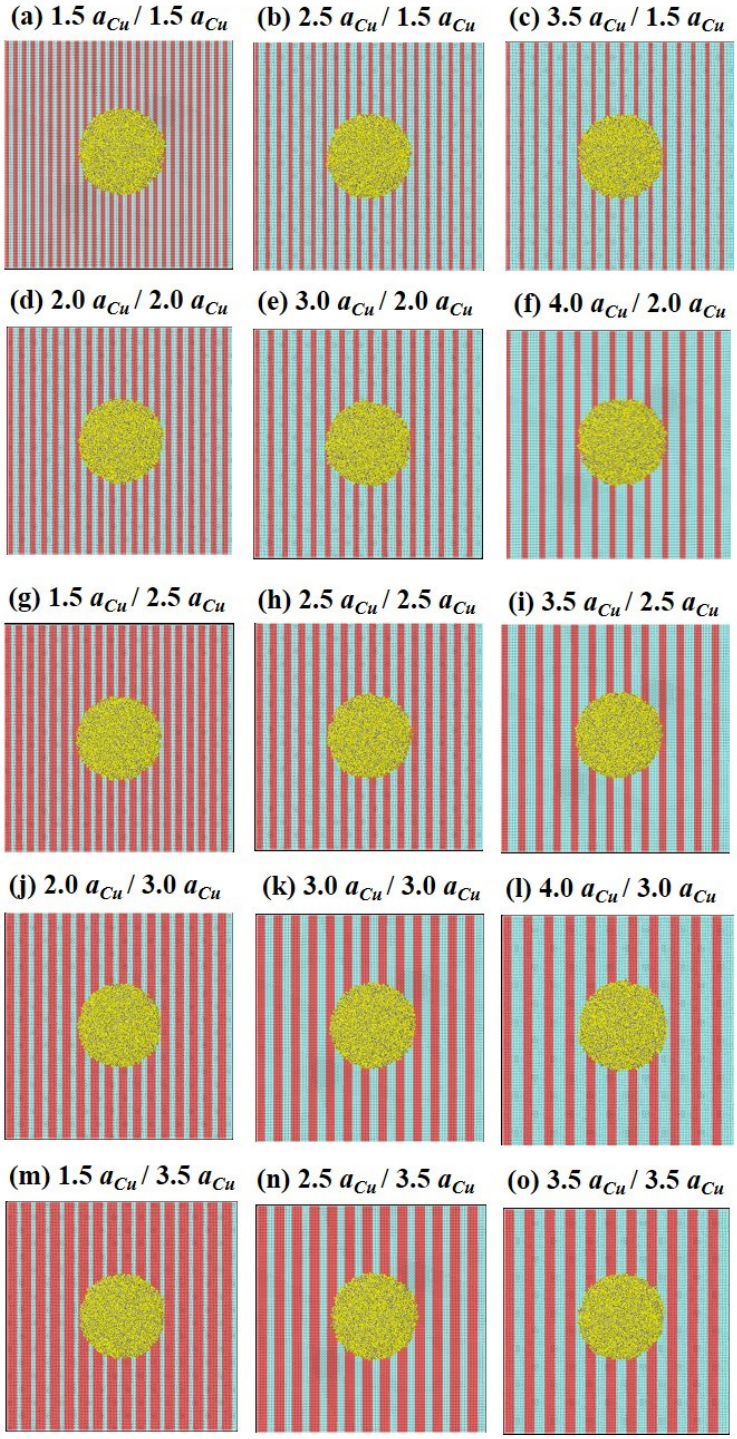

Fig. S2. Top view of ink stripe-pattern surface and water droplet at the beginning of water droplet wetting MD simulation. The descriptions behind the (a-o) are b/a. The a is the stripe width of the ink pattern, and b is the stripe interval width of the printing paper. The red atoms stand for the ink surface, and the azure atoms stand for the printing paper surface. The yellow and blue atoms stand for the oxygen and hydrogen atoms in water, respectively.