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Electronic Supplementary Information (ESI)

Nanocrystalline Cubic Ruthenium Carbide Formation in the Synthesis of Graphene on Ruthenium Ultrathin Films

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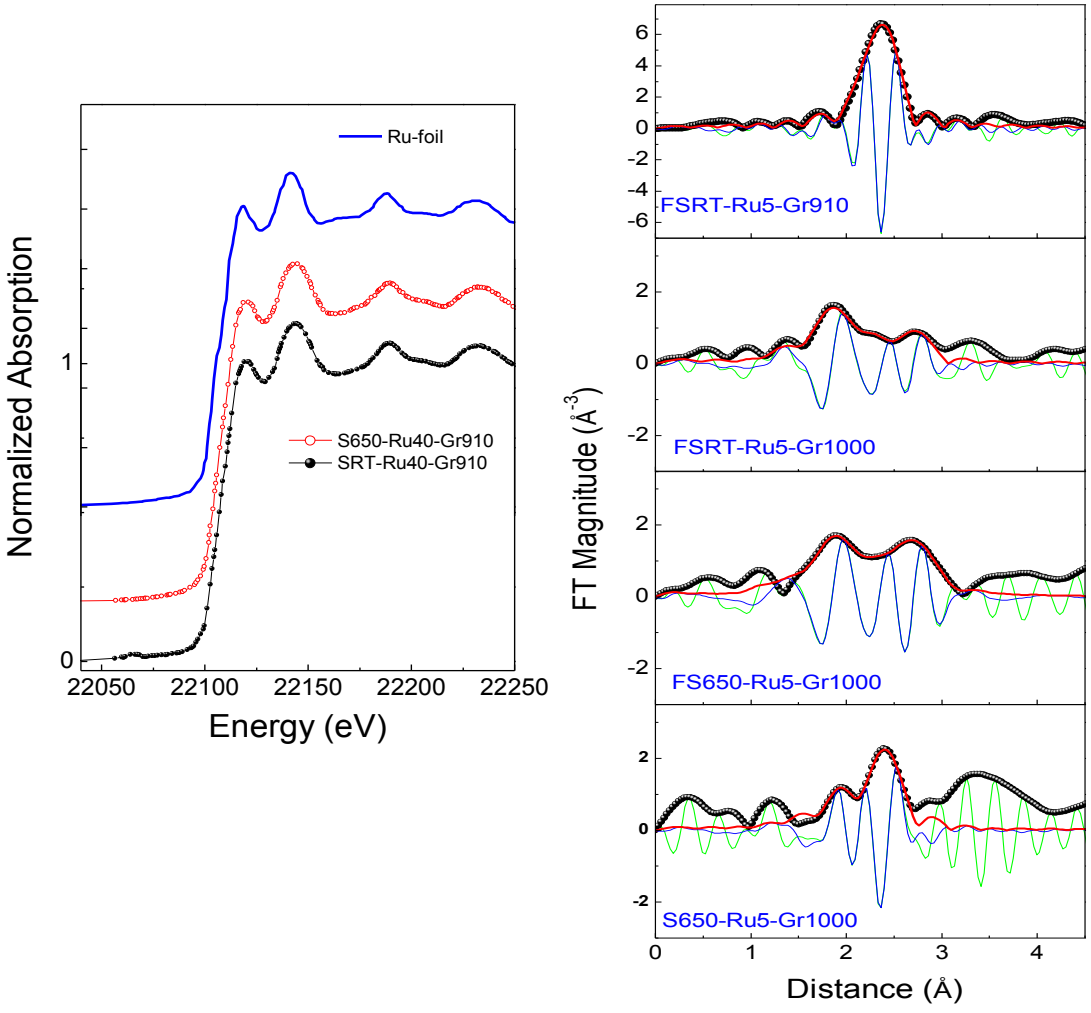

Figure S1. Left panel: Ru XANES spectra of 40 nm thick Ru films grown on sapphire at RT and 650 ºC with graphene synthetized at T_{CVD} = 910 ºC. Ru-foil spectrum is given also for comparison. Right panels: Ru K-edge EXAFS fits of representative samples with graphene. Black dots: FT module experiment; green line: FT imaginary part experiment; red line: FT module simulation; blue line: FT imaginary part simulation. spectrum is given also for comparison.

Table S1. Results obtained from the fits of the EXAFS spectra of samples with and without graphene obtained at different CVD temperatures (T_{CVD}) on fused silica and sapphire. Ru foil results are also included as reference. The asterisks signal the pairs related to the new ruthenium carbide phase.

Sample	***Substrate***	T_S (ºC)	T_{CVD} (ºC)	***pair***	N_j	R_j (Å)	σ^2 ($Å^{-2}$)
Ru foil				Ru-Ru	6.0	2.64	0.0024
				Ru-Ru	6.0	2.73	0.0036
FSRT-Ru5-910	Fused Silica	RT	910	Ru-Ru	6.0±0.3	2.64	0.0017
				Ru-Ru	6.0±0.3	2.74	0.0036
FSRT-Ru5-Gr910	Fused Silica	RT	910	Ru-Ru	5.6±0.3	2.64	0.002
				Ru-Ru	5.6±0.3	2.73	0.0028
FSRT-Ru5-1000	Fused Silica	RT	1000	Ru-Ru	6.0±0.3	2.62	0.0015
				Ru-Ru	6.0±0.3	2.74	0.0024
FSRT-Ru5-Gr1000	Fused Silica	RT	1000	Ru-Ru	3.0±0.5	2.59	0.0098
				*Ru-C	6.0±0.5	2.31	0.0002
				*Ru-Ru	6.0±0.5	2.93	0.0074
FS650-Ru5-1000	Fused Silica	650	1000	Ru-Ru	6.0±0.3	2.64	0.0024
				Ru-Ru	6.0±0.3	2.73	0.0035
FS650-Ru5-Gr1000	Fused Silica	650	1000	Ru-Ru	3.1±0.5	2.57	0.0066
				*Ru-C	6.0±0.5	2.31	0.0010
				*Ru-Ru	7.1±0.5	2.95	0.0074
SRT-Ru40-910	Sapphire	RT	910	Ru-Ru	6.0±0.3	2.60	0.0011
				Ru-Ru	6.0±0.3	2.72	0.0021
S650-Ru40-Gr910	Sapphire	650	910	Ru-Ru	6.0±0.3	2.61	0.0023
				Ru-Ru	6.0±0.3	2.71	0.0013
S650-Ru5-1000	Sapphire	650	1000	Ru-Ru	6.0±0.3	2.64	0.0020
				Ru-Ru	6.0±0.3	2.72	0.0056
S650-Ru5-Gr1000	Sapphire	650	1000	Ru-Ru	4.8±0.5	2.67	0.0048
				*Ru-C	3.2±0.5	2.32	0.0002

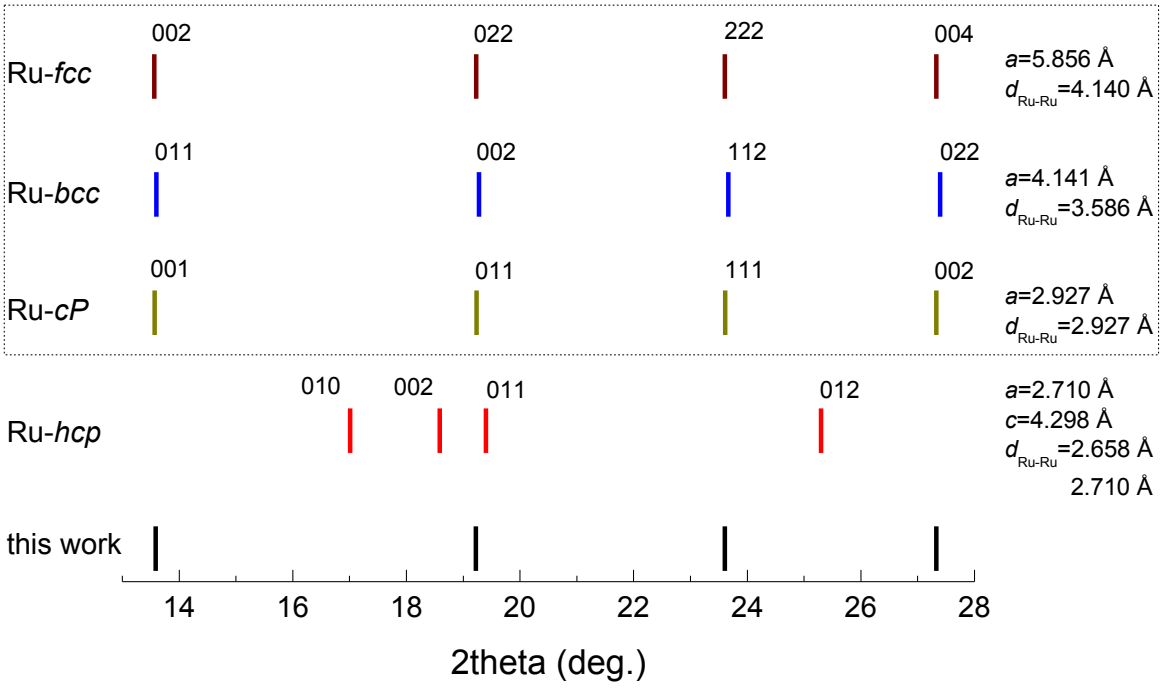

Figure S2. Observed new diffraction maxima (13.58°, 19.22°, 23.60° and 27.33°), (black tick marks) which cannot be indexed considering the hexagonal phase of the metallic ruthenium (red tick marks). Their analysis indicates that these maxima can be indexed by assuming a primitive cubic cell (d_{Ru-Ru} = 2.927 Å), a body-centered cubic cell (d_{Ru-Ru} = 3.586 Å) or a face-centered cubic cell (d_{Ru-Ru} = 4.140 Å), dark yellow, blue and wine tick marks, respectively. However, only the primitive cubic (*cP*) cell is compatible with the EXAFS Ru-Ru and Ru-C interatomic distances (d_{Ru-Ru} = 2.93 Å and d_{Ru-C} = 2.31 Å). Moreover, Ru-Ru distances resulting from the fits to *fcc* and *bcc* structures (4.140 Å and 3.586 Å) are not realistic values.

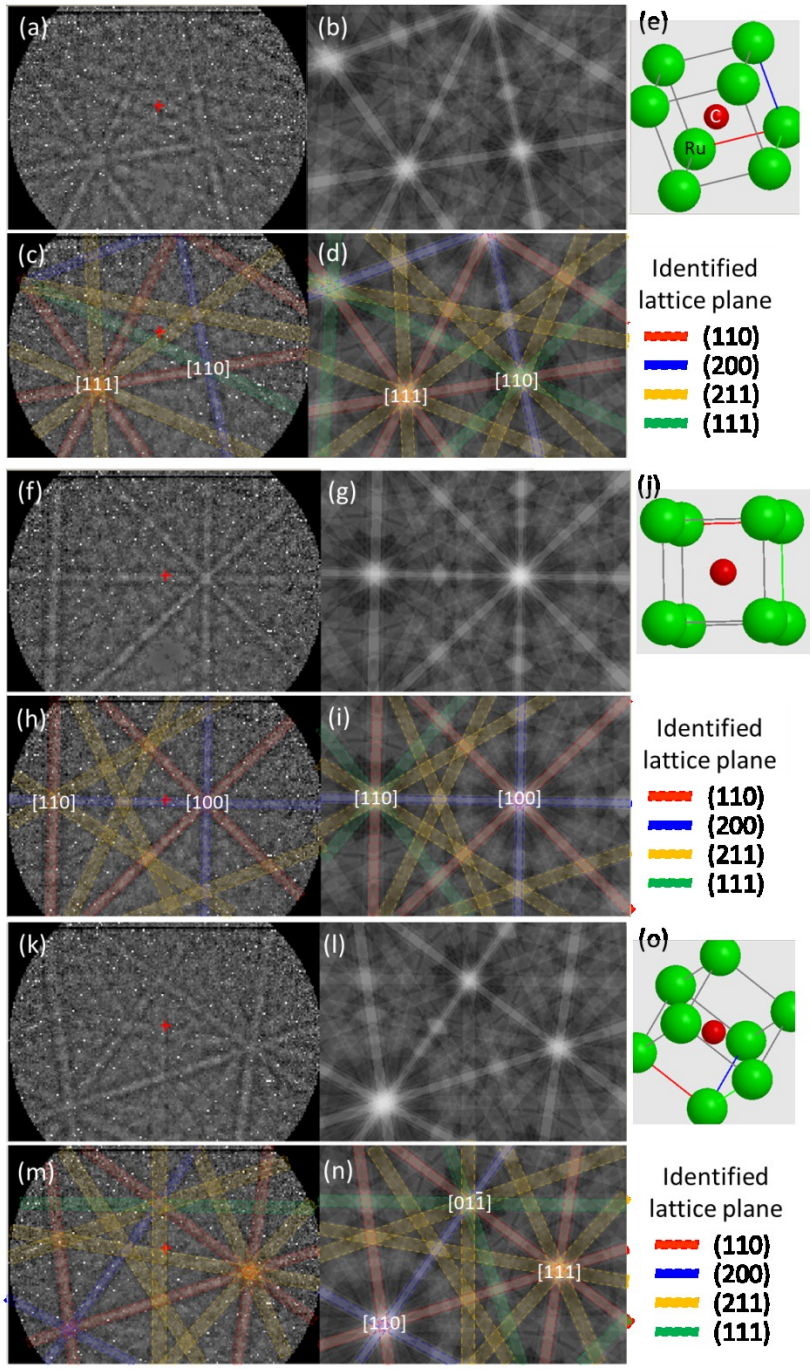

Figure S3. (a, b, f, g, k and l) Experimental EBSD patterns recorded at three different RuC grains, and comparison with the simulated Kikuchi bands for a cubic phase with lattice parameter of 2.927 Å, and crystalline orientation according to sketches shown in (e, j and o) respectively. (c, d, h, i, m and n) Same as before with overlapped low-index lattice planes and poles. Note that only clearly visible bands have been overlapped in the experimental patterns.