INPUT TO MIK CODE – VERIFICATION WITH TODD ALLEN PAPERS

BLUE – checked but different

YELLOW – checked and same

GREEN – doesn’t matter, or user-supplied

4.0 18.0 2018.0 16 14 20 ! R1,R2,RF,N1,N2,N3

! distance to mesh groups, no. of points in mesh groups

1.0E-09 1.0E-09 ! H0,EPS

! input time step to gear, error control parameter

1.40000000e-06 1.00000000 1.00000000 1.0 ! DISPRT,ETAV,ETAI,DOSE

! peak displ rate, v/i production efficiency, dose

360.00000000 ! TEMPC

! peak temperature

0.2100000 0.0900000 ! CONCB,CONCC

! concentration of B, C

1.00000e+14 9.10000e+28 3.50000e-10 ! DISL,NAT,LAMBDA

! peak disloc density, no. density, jump distance

0.785 0.668 0.872 0.660 ! FAV,FBV,FCV,FI -- 0.44???

! jump correlation factors (A,B,C,interstitial)

1.80000000 3.20000000 1.00000000 ! WAV,WBV,WCV -- 1.6 (1.4) ,2.4 (2.3),1.0 or

! 1.86666666666,3.3333333333

! relative vac jump frequency ratios (A,B,C)

1.00000000 1.00000000 1.00000000 ! WAI,WBI,WCI

! relative int jump frequency ratios (A,B,C)

-4.28000000-4.21000000-4.44000000 ! ECOHA,ECOHB,ECOHC -- -4.28,-4.10,-4.44

! cohesive energies

0.90000000 0.90000000 0.90000000 1.00000000 ! EMIA,EMIB,EMIC,SV

! int migration energies, vac formation enthalpy

1.28000000 0.97000000 1.04000000 ! EMA,EMB,EMC

! pure element [vac] migration energies

1.40000000 1.60000000 1.79000000 1.40000000 ! EFA,EFB,EFC,EFGB

! pure element [vac] form’n energy, GB formation energy

0.00300000-0.00100000 0.00500000 ! EORDAB,EORDAC,EORDBC

! ordering energies

1.5e+13 1.5e+12 ! NUOV,NUOI

! debye frequencies

1.00000000 12.00 1.00 1.00 ! AL,Z,BIASV,BIASI

! thermo factor, neighbor atoms, disloc bias for v/i

1.0E-00 1.0E+01 5.0E+02 1.0e+03 5.0e+03 1.4e+04 ! TOUTPT(I),I=1,20

5.0E+04 7.1E+04 1.0E+05 1.4e+05 3.6e+05 4.3e+05 !

7.1E+05 2.1E+06 2.2E+06 2.3e+06 5.0e+06 7.0e+07 !

1.0e+08 0.0e+00 !

! user-required output times

N ! FRAC

! indicates whether profiles will be used

1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 ! TFRAC(I),I=1,NSTEP-1

1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 ! fraction of max temperature

1.0000 1.0000 1.0000 !

1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 ! CAFRAC(I),I=1,NSTEP

1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 ! fraction of peak atom A

1.0000 1.0000 1.0000 !

0.1231 0.2991 0.3912 0.4573 0.5100 0.6988 ! CBFRAC(I),I=1,NSTEP

0.8144 0.8969 0.9613 1.0150 1.0000 1.0000 ! fraction of peak atom B

1.0000 1.0000 1.0000 !

1.1670 1.1334 1.1160 1.1033 1.0933 1.0574 ! CCFRAC(I),I=1,NSTEP

1.0354 1.0196 1.0074 0.9971 1.0000 1.0000 ! fraction of peak atom C

1.0000 1.0000 1.0000 !

1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 ! DFRAC(I),I=1,NSTEP

1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 ! fraction of peak damage

1.0000 1.0000 1.0000 !

1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 ! SFRAC(I),I=1,NSTEP

1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 ! fraction of max disloc density

1.0000 1.0000 1.0000 !