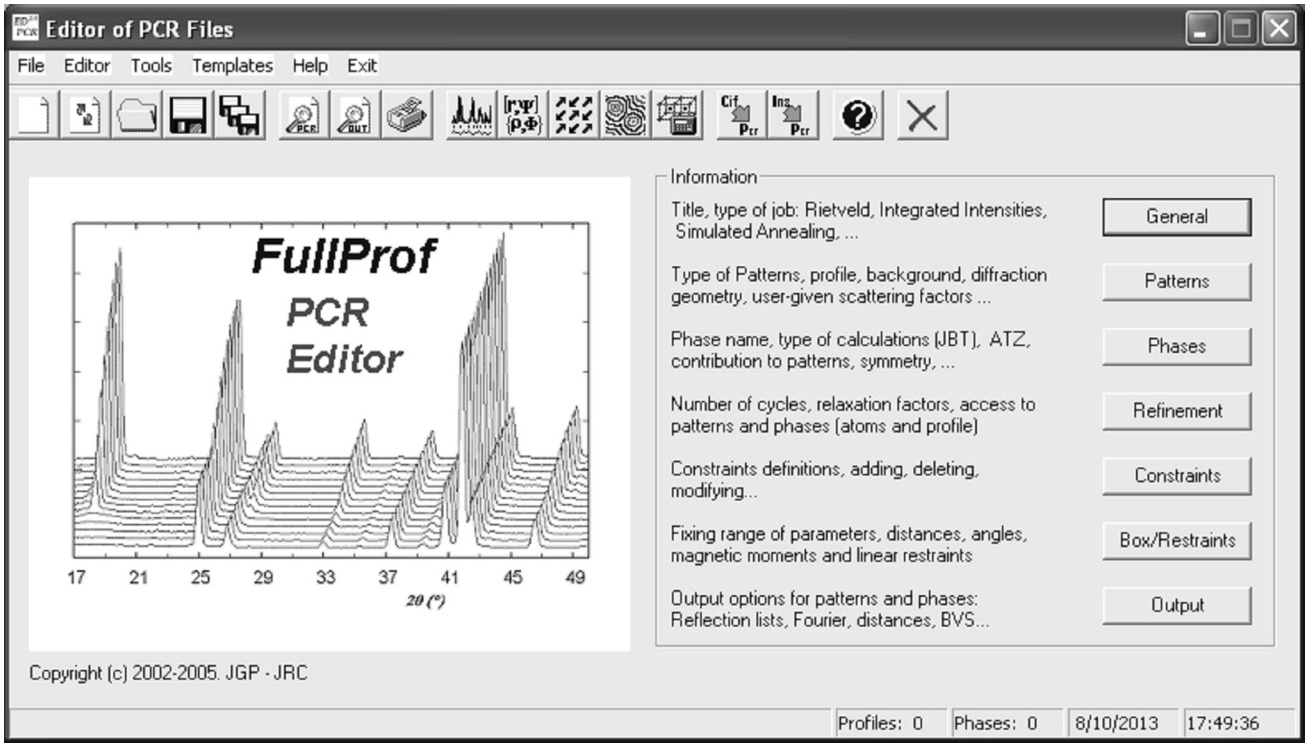
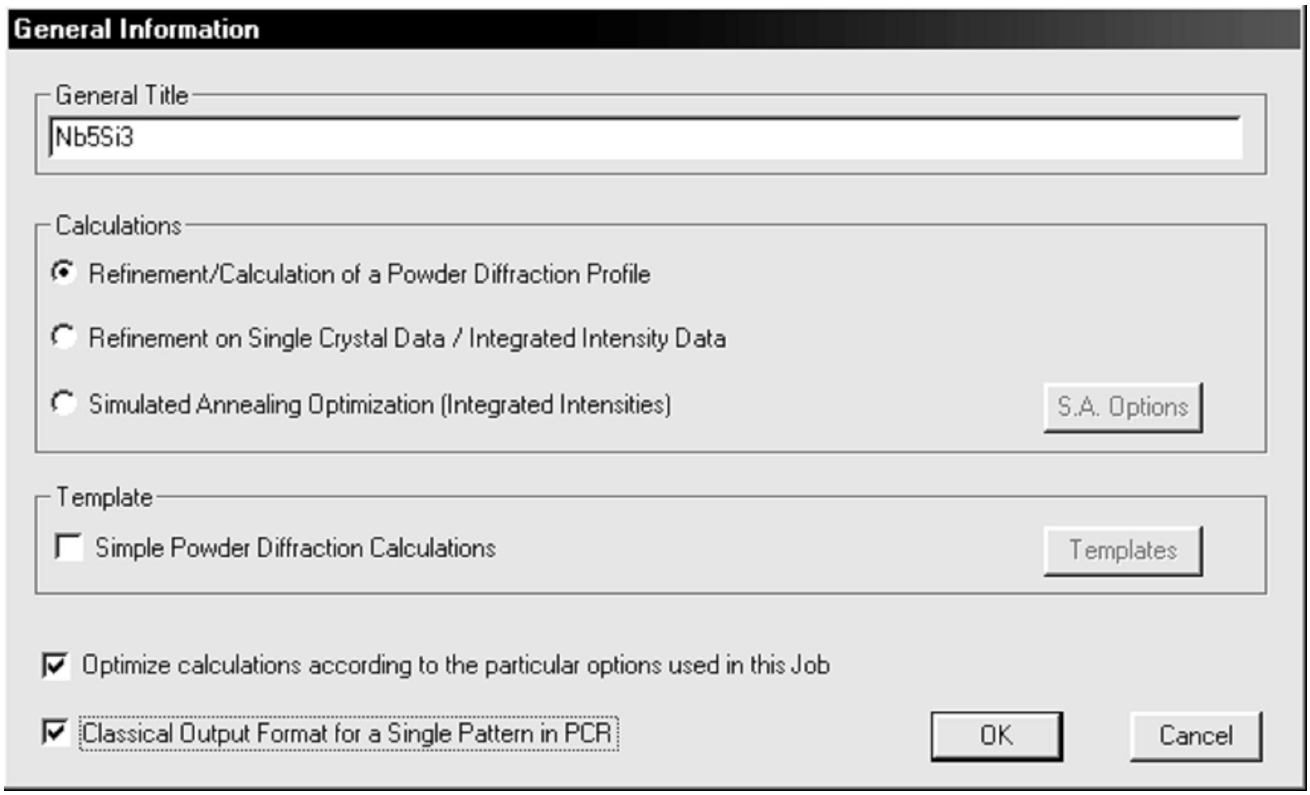
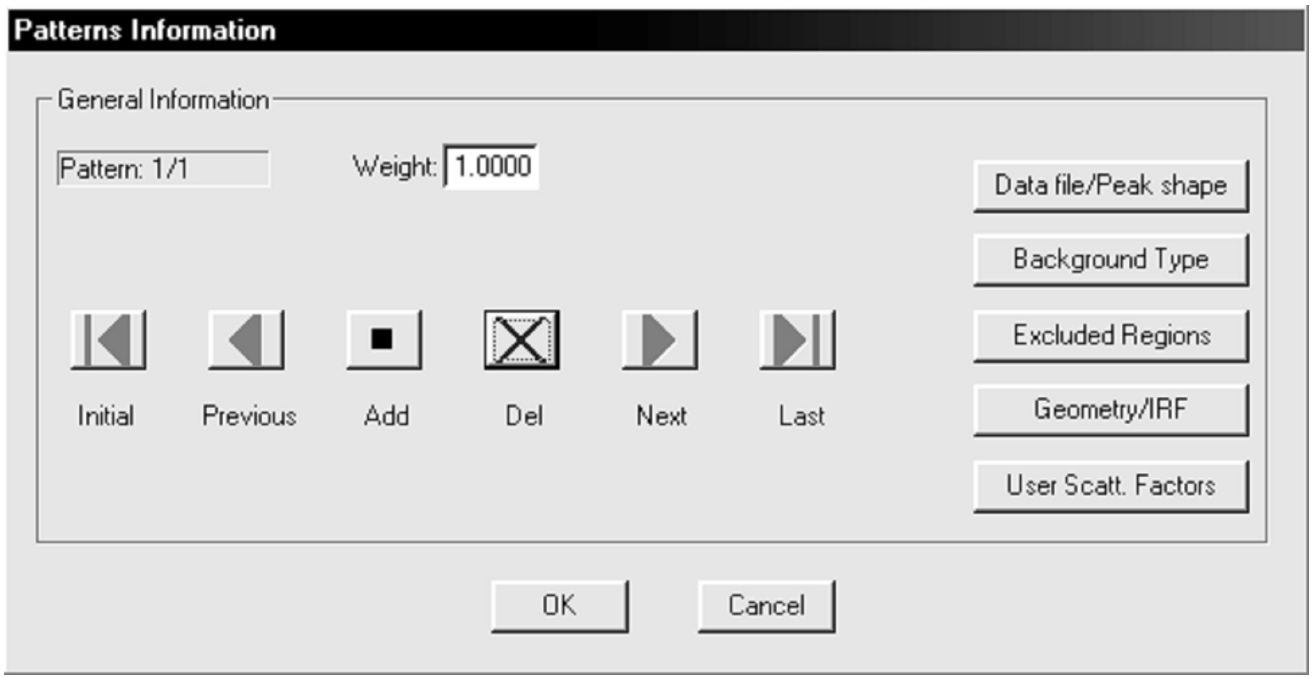
FullProf



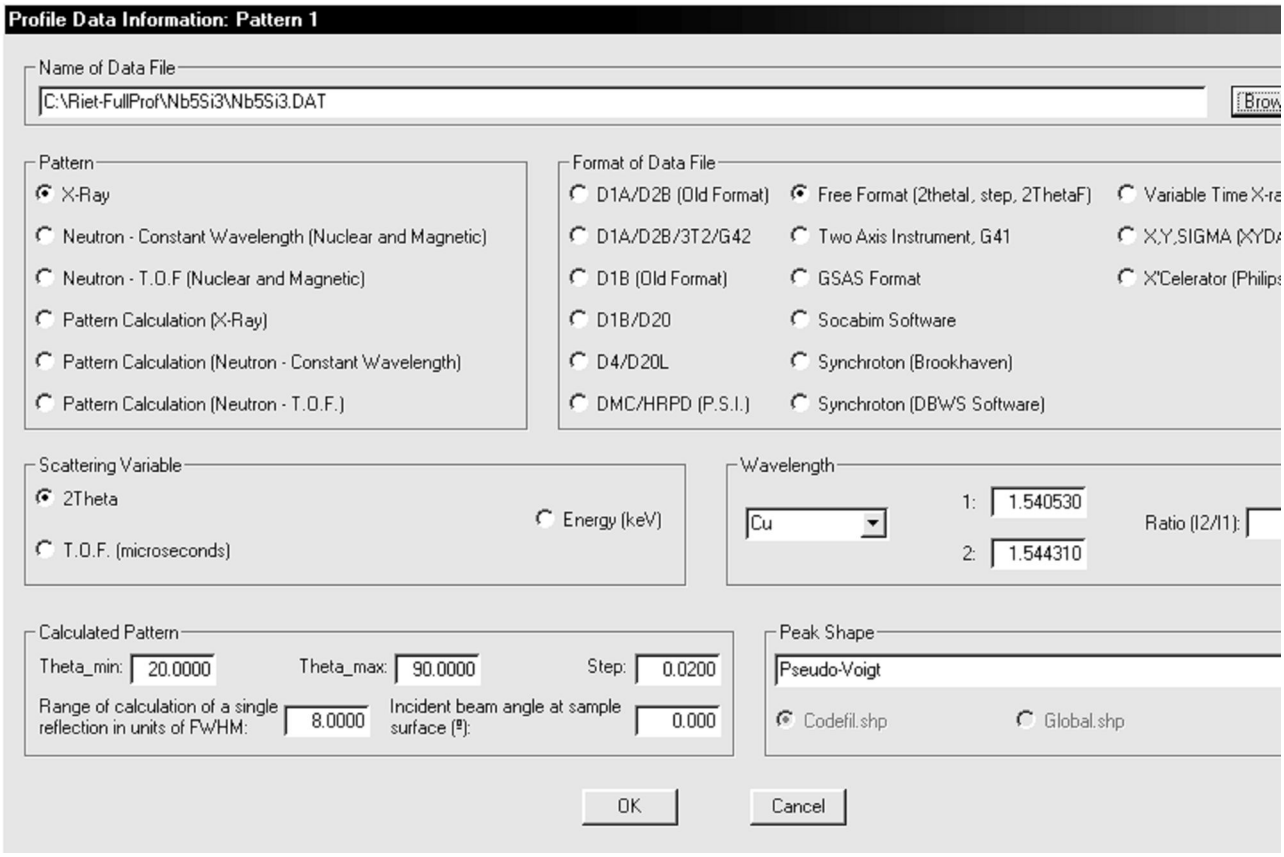
Pasta: General



Pasta: Patterns



Pasta: Patterns / **Sub-pasta:** Data file/Peak shape



Formato do arquivo de dados:

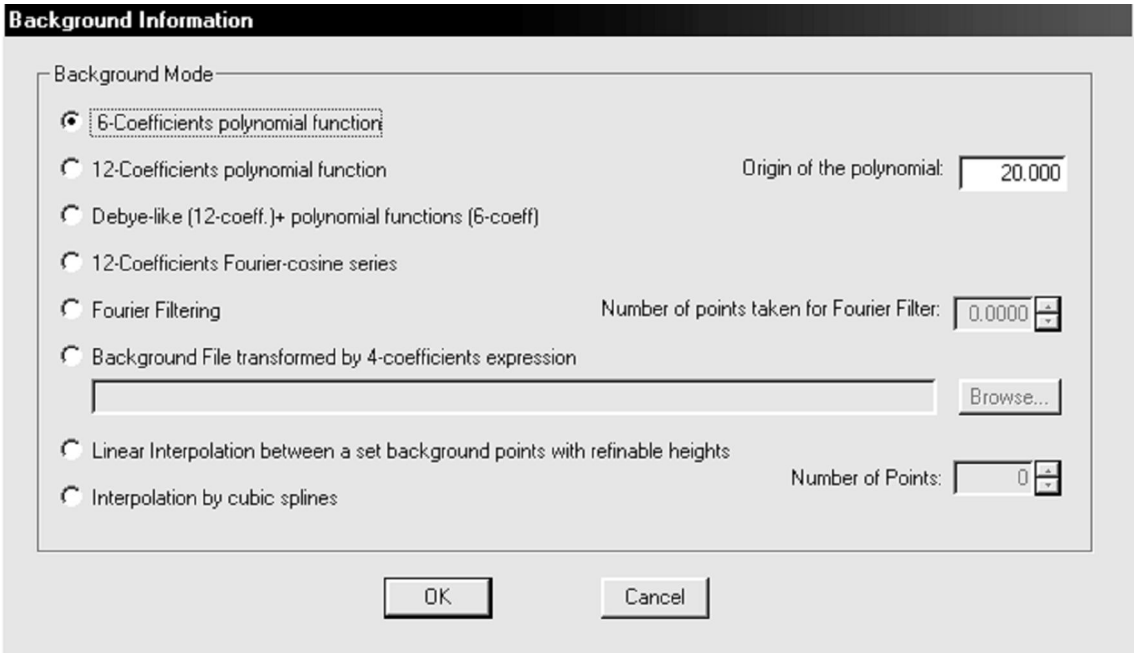
Free format: Nb5Si3.dat

1ª linha: âng. inicial□passo angular□âng. final

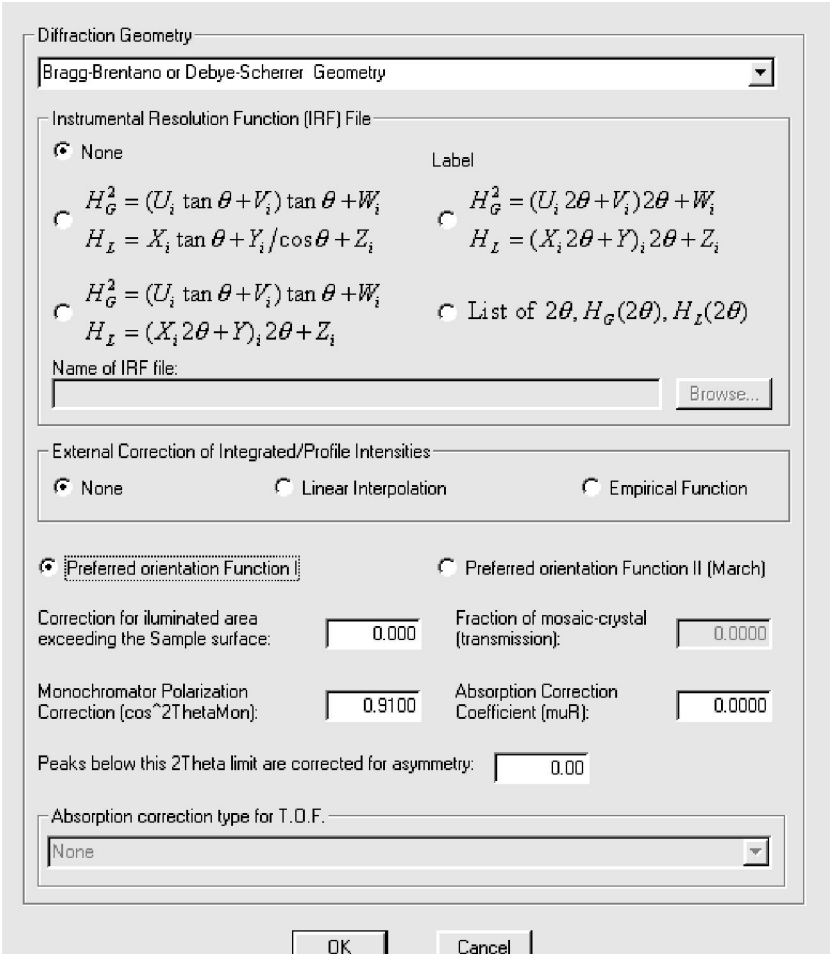
2ª linha até Nª linha: <u>uma coluna</u> contendo somente a intensidade.

Obs: □ = espaço

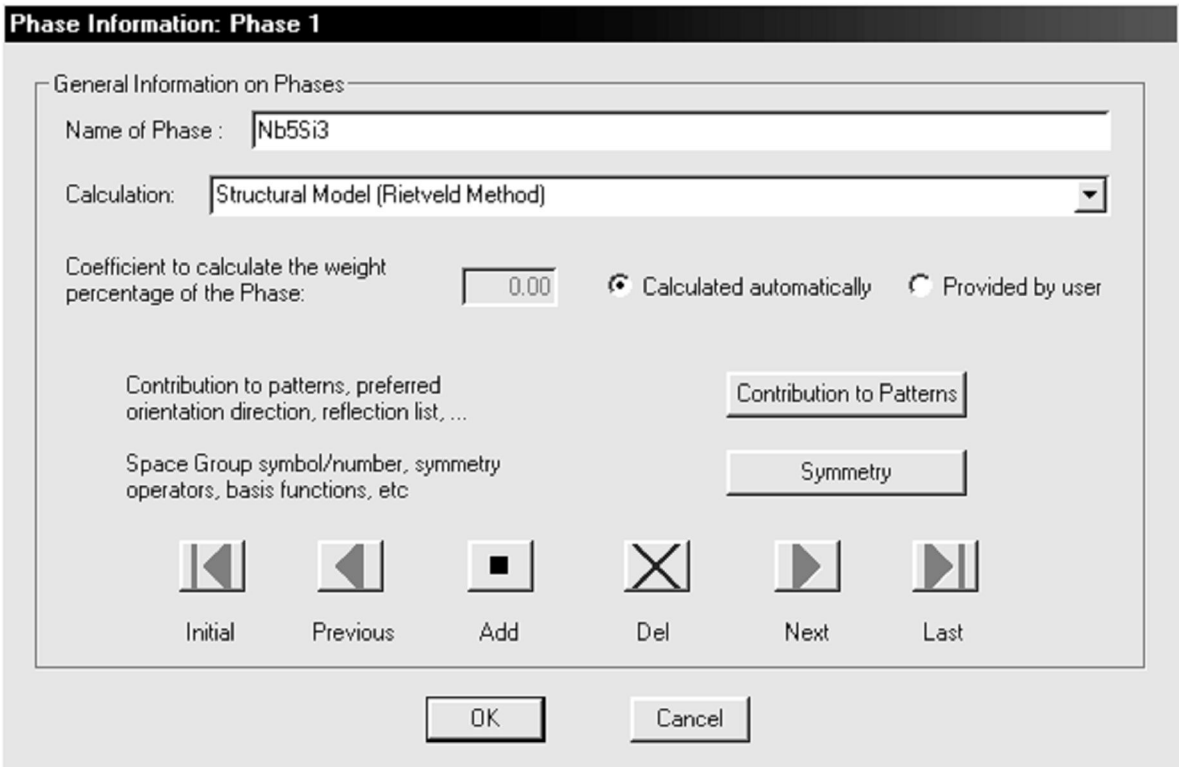
Pasta: Patterns / **Sub-pasta:** Background Type



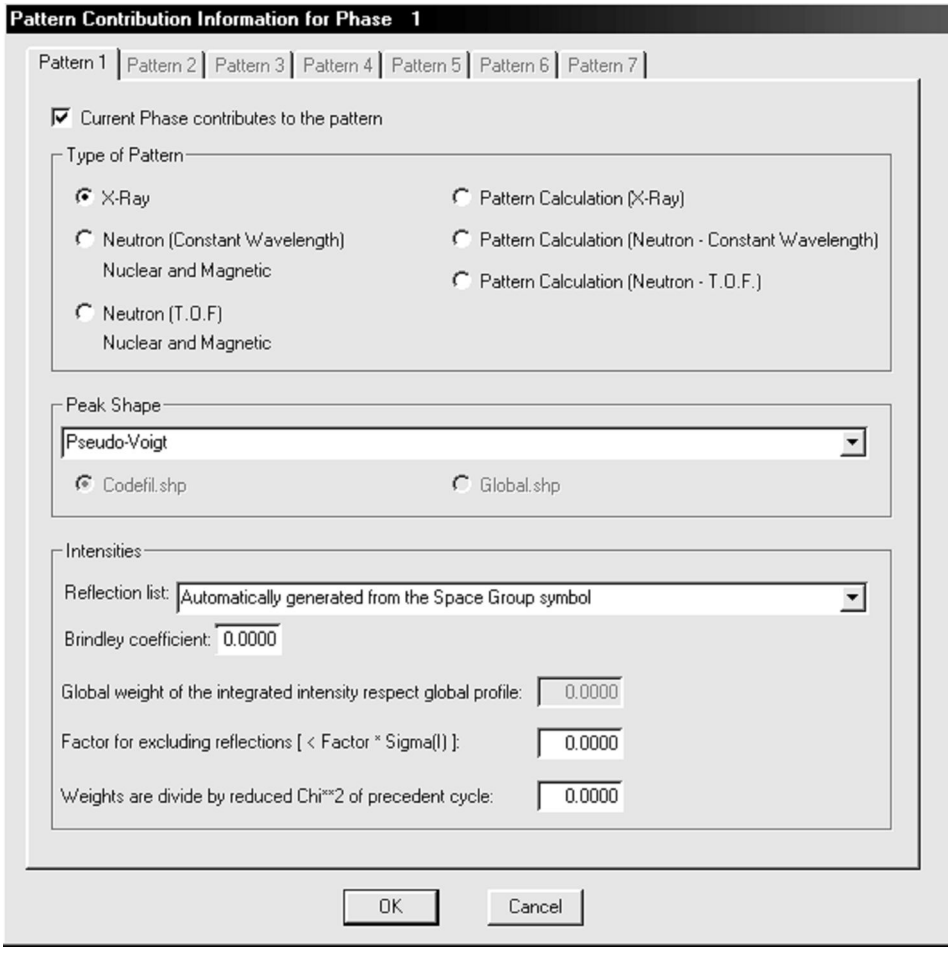
Pasta: Patterns / **Sub-pasta:** Geometry / IRF



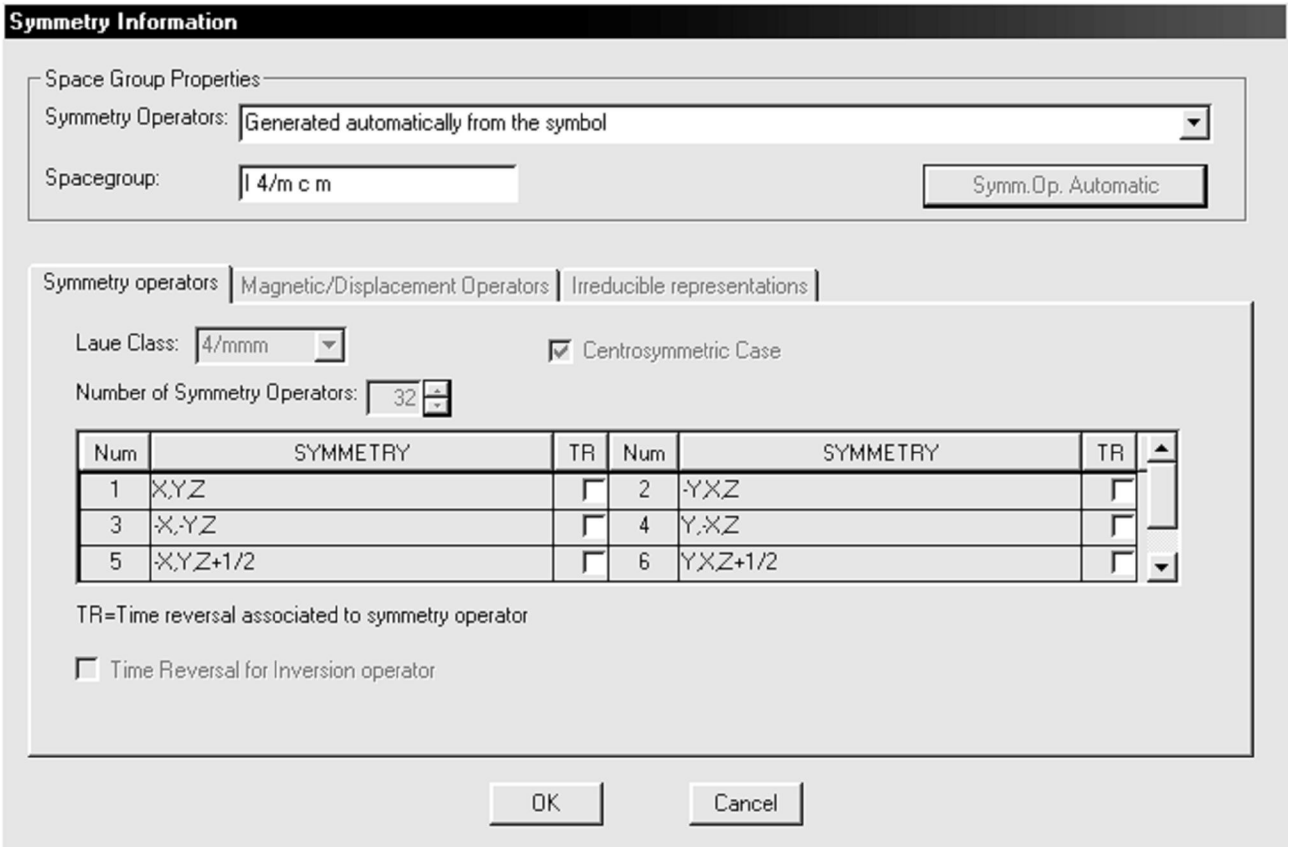
Pasta: Phases



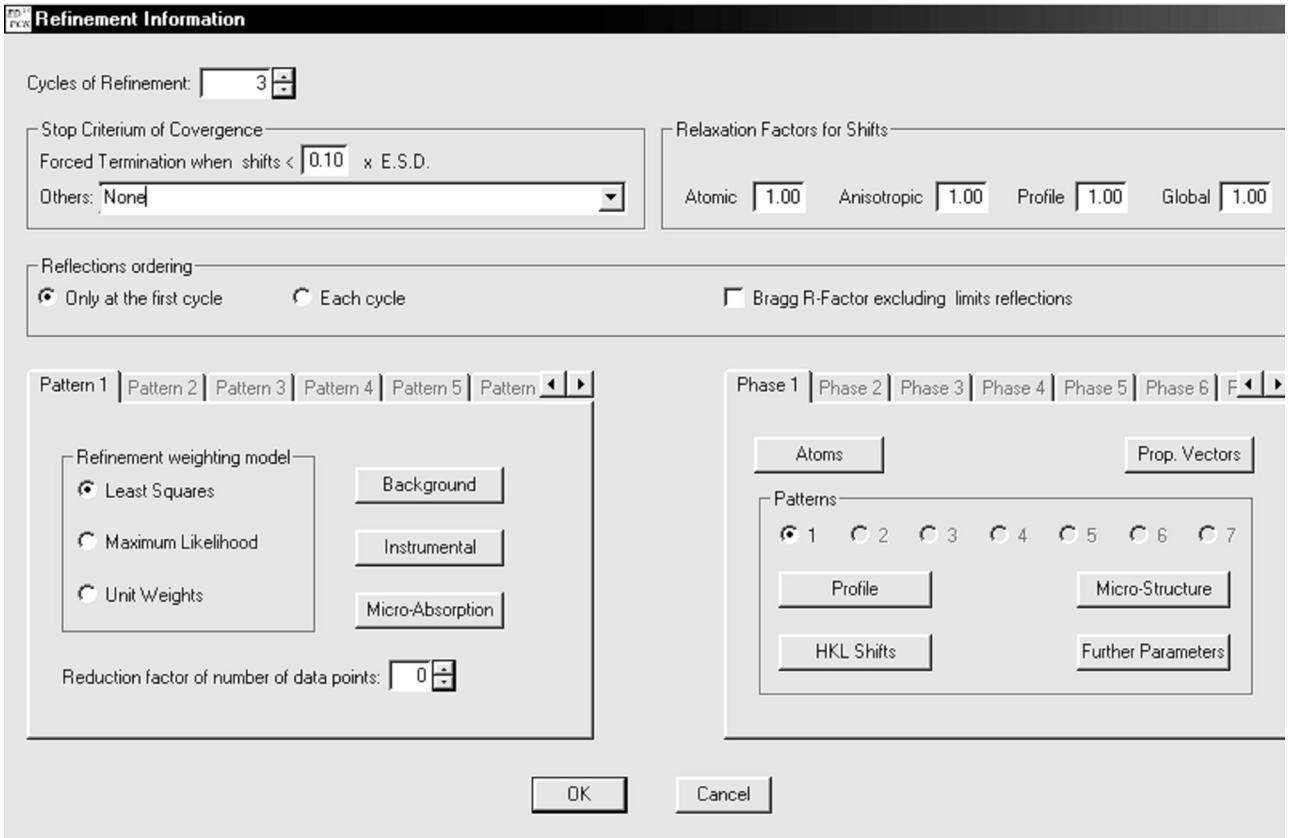
Pasta: Phases / **Sub-pasta:** Contribution to Patterns



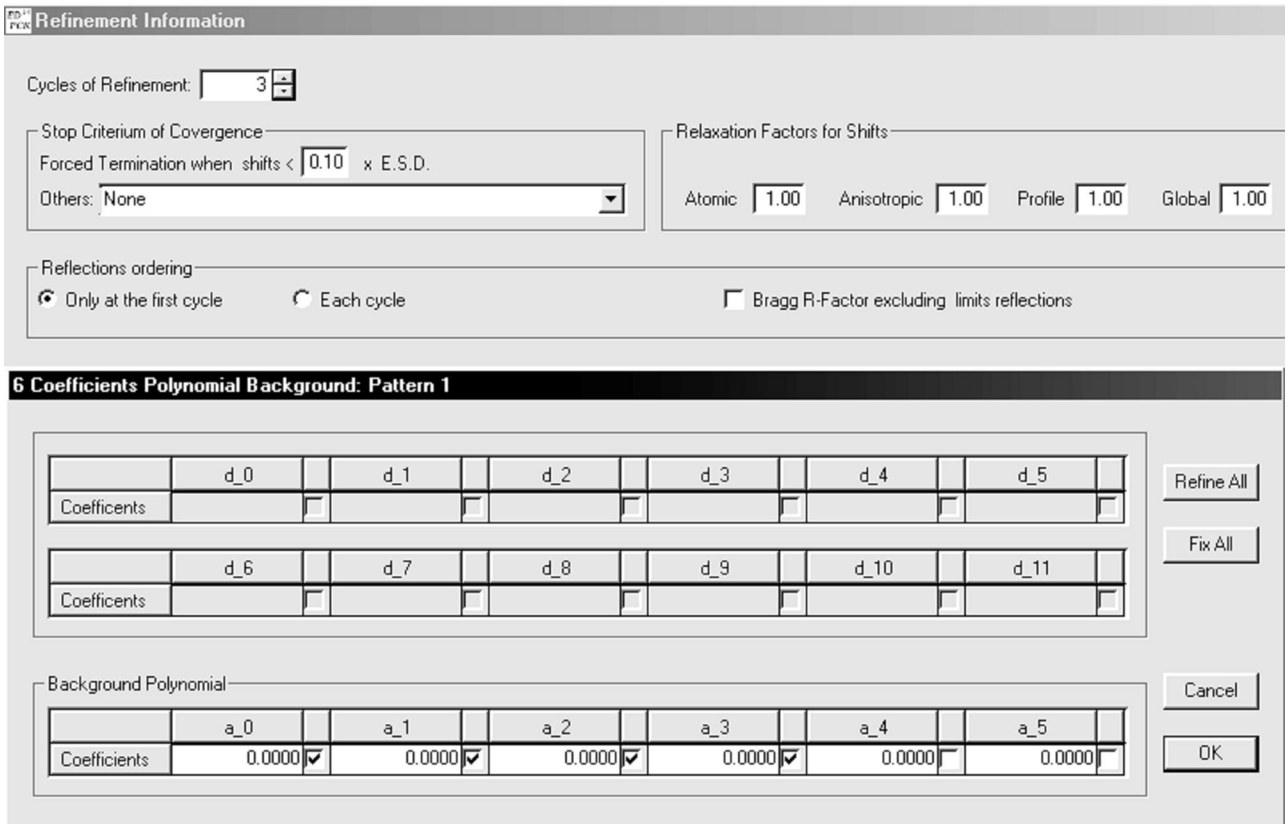
Pasta: Phases / **Sub-pasta:** Symmetry



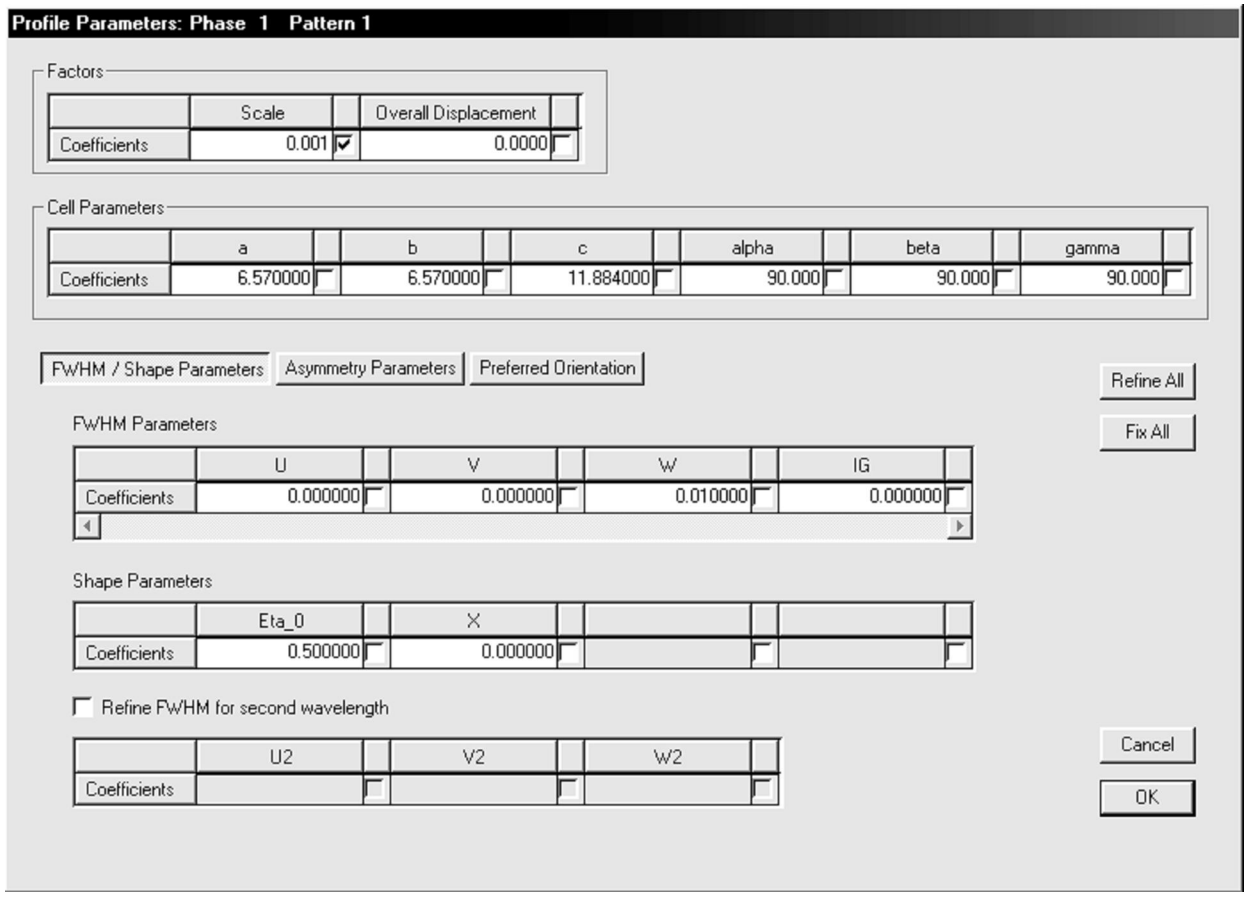
Pasta: Refinement



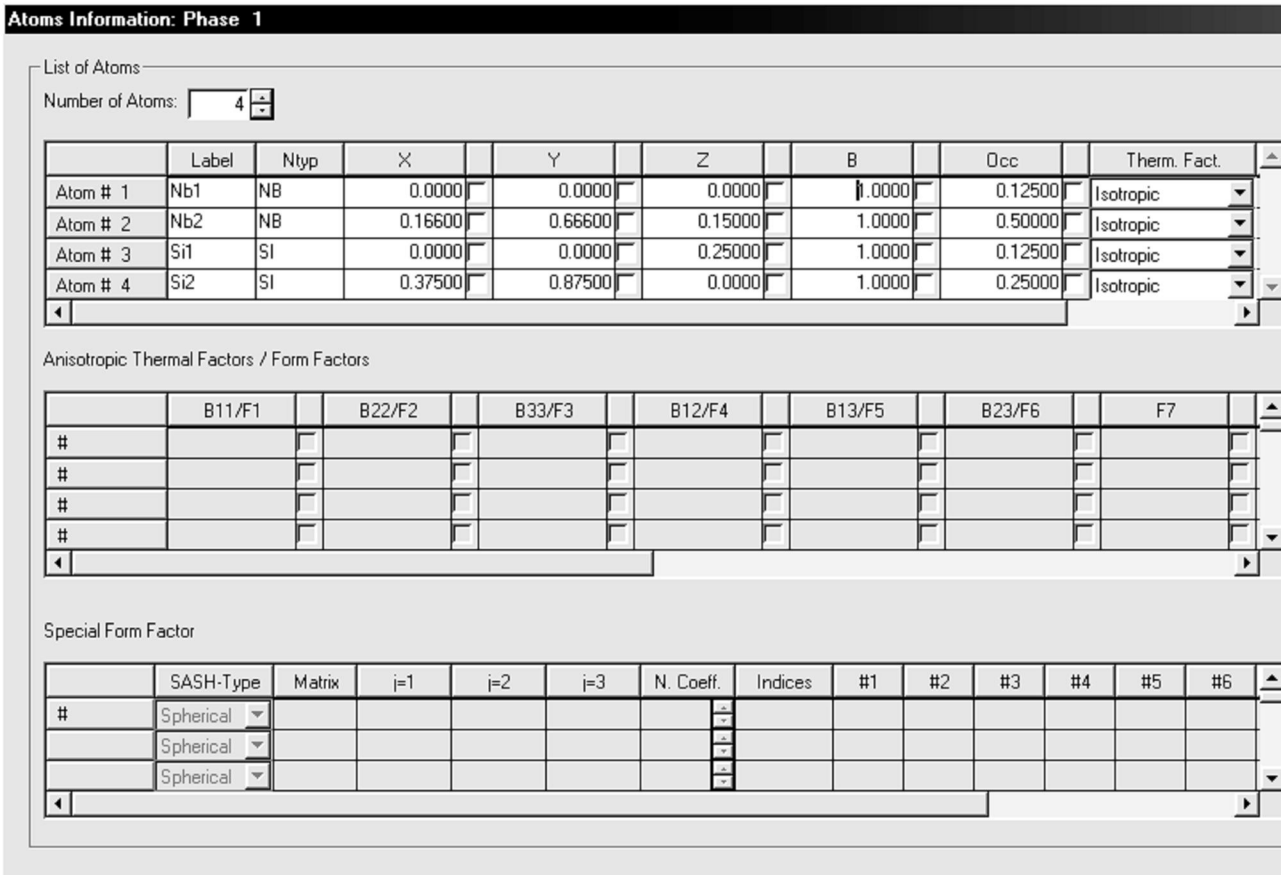
Pasta: Refinement / **Sub-pasta:** Background



Pasta: Refinement / **Sub-pasta:** Profile



Pasta: Refinement / **Sub-pasta:** Atoms



átomo	posição Wyckoff	x	y	z	B(Å^2)	Occ (ocupação) (*)
Nb 1	4(c)	0	0	0	1	4/32 = 0.125
Nb 2	16(l)	x	x+1/2	z	1	16/32 = 0.5
Si 1	4(a)	0	0	1/4	1	4/32 = 0.125
Si 2	8(h)	x	x+1/2	0	1	8/32 = 0.25

x(Nb2)=0,166 z(Nb2)=0,15 x(Si2)=0,375

Grupo espacial: I 4/m c m: posição geral: 32(m)

(*) Obs: Para calcular a ocupação, dividir a posição Wyckoff pelo número de posição geral.

Pasta: Refinement / **Sub-pasta:** Instrumental